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(54) Title: METAL CHELATES

(57) Abstract: A photovoltaic device which uses a metal chelate as the photovoltaic element.



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## Metal Chelates

The present invention relates to photovoltaic devices and elements useful in such devices.

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Photovoltaic devices, i.e. solar cells, are capable of converting solar radiation into useable electrical energy. The energy conversion occurs as a result of what is well known in the solar cell field as the photovoltaic effect. Solar radiation impinging on a solar cell and absorbed by an active region generates electrons and holes. The

10 electrons and holes are separated by a built-in electric field, for example a rectifying junction, in the solar cell. This separation of electrons and holes results in the generation of an electrical current as explained below. For example, a built-in electric field can be generated in a solar cell by an active semiconductor layer with regions of P-type, intrinsic and N-type hydrogenated amorphous silicon. A built-in electric field

15 can also be generated in a solar cell by, for example, a Schottky barrier. The electrons generated at the metal (Schottky barrier) semiconductor body junction flow towards the semiconductor body.

20

A typical simple photovoltaic solar cell comprises an electrically conductive substrate layer; a semiconductor body deposited upon said substrate layer and a transparent conductive layer over at least a portion of said semiconductor body for facilitating collection of electrical current produced by the photovoltaic cell.

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The electrons generated in the intrinsic region, by absorption of solar radiation of the appropriate bandgap, produce electron-hole pairs. The separation of the electron-hole pairs with the electrons flowing toward the region of N-type conductivity, and the holes flowing toward the region of P-type conductivity, creates the photovoltage and photocurrent of the cell.

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The photocurrent output of a solar cell is maximized by increasing the total number of photons of differing energy and wavelength which are absorbed by the

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semiconductor material. The solar spectrum roughly spans the region of wavelengths from about 300 nanometers to about 2200 nanometers, which corresponds to from about 4.2 eV to about 0.59 eV, respectively. The portion of the solar spectrum which is absorbed by the solar cell is determined by the size of the bandgap energy of the semiconductor material. In the past, solar cells were fabricated from single crystal materials such as gallium arsenide, which has a bandgap energy of about 1.45 eV, or crystalline silicon, C-Si, which has a bandgap energy of about 1.1 eV. Solar radiation having an energy less than the bandgap energy is not absorbed by the semiconductor material, and thus does not contribute to the generation of the photocurrent output of the cell.

Semiconductor materials such as GaAs and C-Si have been utilized together in solar cells to increase the overall conversion of solar energy into electrical energy. However, problems are encountered when different semiconductor materials are used in the same solar cell. One solution to the problem of fabricating a solar cell structure with different semiconductor materials was to use filters to reflect light of the appropriate wavelength onto a solar cell of the first material and transmit the non-absorbed light to a cell of the second semiconductor material. A second solution used semiconductor materials of differing bandgaps which could be epitaxially grown on one another, such as aluminum gallium arsenide, gallium arsenide, and gallium phosphide structures. Both these systems have been loosely called tandem junction solar cells. A third alternative was to stack individual solar cells of differing bandgap energies and connect the cells in series. These three alternatives are either cumbersome, expensive and/or bulky. A description of photovoltaic cells and their operation is disclosed in a paper by Jean-Michel Nunzi in C.R.Physique 3 (2002) 523-542.

We have found that a photovoltaic device can be made using metal chelates such as a rare earth or non rare earth metal chelate or a mixture of rare earth metal chelates as the photovoltaic element in place of the prior art semi conductors.

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Rare earth chelates are known which fluoresce in ultra violet radiation and A. P. Sinha (Spectroscopy of Inorganic Chemistry Vol. 2 Academic Press 1971) describes several classes of rare earth chelates with various monodentate and bidentate ligands.

5

Group III A metals and lanthanides and actinides with aromatic complexing agents have been described by G. Kallistratos (Chimica Chronika, New Series, 11, 249-266 (1982)). This reference specifically discloses the Eu(III), Tb(III), U(III) and U(IV) complexes of diphenyl-phosponamidotriphenyl-phosphoran.

10

EP 0556005A and 0744451A also disclose fluorescent chelates of transition or lanthanide or actinide metals.

15

Patent application WO98/58037 describes a range of lanthanide complexes which can be used in electroluminescent devices which have improved properties and give better results. Patent Applications PCT/GB98/01773, PCT/GB99/03619, PCT/GB99/04030, PCT/GB99/04024, PCT/GB99/04028, PCT/GB00/00268 describe electroluminescent complexes, structures and devices using rare earth chelates.

20

Hitherto such rare earth metal chelates have not been used in photovoltaic devices.

According to the invention there is provided a photovoltaic device comprising a metal chelate as the photovoltaic element.

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The invention also provides a photovoltaic device which comprises sequentially (i) a first electrode comprising a metal, (ii) the photovoltaic element and (iii) a second electrode in which the photovoltaic element comprises a metal chelate.

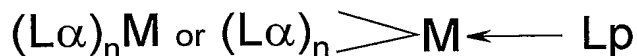
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By photovoltaic element is meant a compound which will generate electrons and holes when exposed to light.

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The metal chelates can absorb light of a specific wavelength or wavelengths depending on the metal and ligands used and, as the photocurrent output of a solar cell is maximized by increasing the total number of photons of differing energy and wavelength which are absorbed by the semiconductor material, by having a plurality of layers of different metal chelates which absorb light at different wavelengths, a wide range of the visible spectrum can be used. Metal chelates can also absorb light in the infra-red, ultra-violet or shorter wavelengths so improving the utilisation of sunlight and increasing the power achievable by a solar cell. Alternatively there can be several layers of metal chelates which absorb light in different parts of the spectrum.

The preferred metal chelates useful in the present invention have the formula



where  $L\alpha$  and  $Lp$  are organic ligands,  $M$  is a metal and  $n$  is the valence state of the metal  $M$  and in which the ligands  $L\alpha$  are the same or different.

There can be a plurality of ligands  $Lp$  which can be the same or different.

For example  $(L_1)(L_2)(L_3)(L...)M (Lp)$  where  $M$  is a metal e.g. rare earth, transition metal, lanthanide or an actinide and  $(L_1)(L_2)(L_3)(L...)$  are the same or different organic complexes and  $(Lp)$  is a neutral ligand. The total charge of the ligands  $(L_1)(L_2)(L_3)(L...)$  is equal to the valence state of the metal  $M$ . Where there are 3 groups  $L\alpha$  which corresponds to the III valence state of  $M$  the complex has the formula  $(L_1)(L_2)(L_3)M (Lp)$  and the different groups  $(L_1)(L_2)(L_3)$  may be the same or different.

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Lp can be monodentate, bidentate or polydentate and there can be one or more ligands Lp.

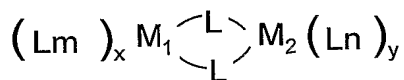
Preferably M is a metal ion having an unfilled inner shell and the preferred metals are selected from Sm(III), Eu(II), Eu(III), Tb(III), Dy(III), Yb(III), Lu(III), Gd (III),  
 5 Gd(III) U(III), Tm(III), Ce (III), Pr(III), Nd(III), Pm(III), Dy(III), Ho(III), Er(III) and more preferably Eu(III), Tb(III), Dy(III), Gd (III).

Further compounds which can be used in the present invention are of general formula  
 10  $(L\alpha)_n M_1 M_2$  where  $M_1$  is the same as M above,  $M_2$  is a non rare earth metal,  $L\alpha$  is as above and  $n$  is the combined valence state of  $M_1$  and  $M_2$ . The complex can also comprise one or more neutral ligands Lp so the complex has the general formula  $(L\alpha)_n M_1 M_2 (Lp)$ , where Lp is as above. The metal  $M_2$  can be any metal which is not a rare earth, transition metal, lanthanide or an actinide; examples of metals which can  
 15 be used include lithium, sodium, potassium, rubidium, caesium, beryllium, magnesium, calcium, strontium, barium, copper (I), copper (II), silver, gold, zinc, cadmium, boron, aluminium, gallium, indium, germanium, tin (II), tin (IV), antimony (II), antimony (IV), lead (II), lead (IV) and metals of the first, second and third groups of transition metals in different valence states e.g. manganese, iron, ruthenium,  
 20 osmium, cobalt, nickel, palladium(II), palladium(IV), platinum(II), platinum(IV), cadmium, chromium. titanium, vanadium, zirconium, tantalum, molybdenum, rhodium, iridium, titanium, niobium, scandium, yttrium.

For example  $(L_1)(L_2)(L_3)(L_{..})M (Lp)$  where M is a rare earth, transition metal,  
 25 lanthanide or an actinide and  $(L_1)(L_2)(L_3)(L_{...})$  and  $(Lp)$  are the same or different organic complexes.

Further organometallic complexes which can be used in the present invention are binuclear, trinuclear and polynuclear organometallic complexes e.g. of formula  
 30  $(Lm)_x M_1 \leftarrow M_2(Ln)_y$  e.g.

- 6 -

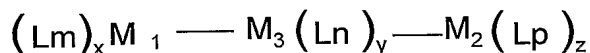


where L is a bridging ligand and where  $M_1$  is a rare earth metal and  $M_2$  is  $M_1$  or a non rare earth metal, Lm and Ln are the same or different organic ligands  $L\alpha$  as defined above, x is the valence state of  $M_1$  and y is the valence state of  $M_2$ .

In these complexes there can be a metal to metal bond or there can be one or more bridging ligands between  $M_1$  and  $M_2$  and the groups Lm and Ln can be the same or different.

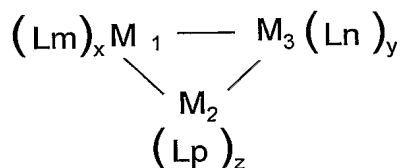
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By trinuclear is meant there are three rare earth metals joined by a metal to metal bond i.e. of formula



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or



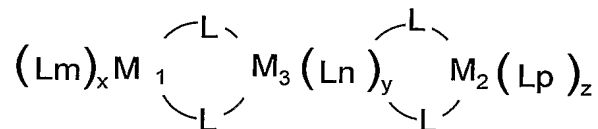
where  $M_1$ ,  $M_2$  and  $M_3$  are the same or different rare earth metals and Lm, Ln and Lp are organic ligands,  $L\alpha$  and x is the valence state of  $M_1$ , y is the valence state of  $M_2$  and z is the valence state of  $M_3$ . Lp can be the same as Lm and Ln or different.

The rare earth metals and the non rare earth metals can be joined together by a metal to metal bond and/or via an intermediate bridging atom, ligand or molecular group.

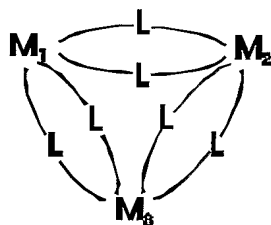
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For example the metals can be linked by bridging ligands e.g.

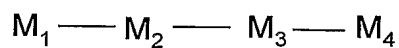


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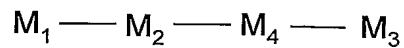
where L is a bridging ligand

10 By polynuclear is meant there are more than three metals joined by metal to metal bonds and/or via intermediate ligands

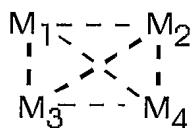


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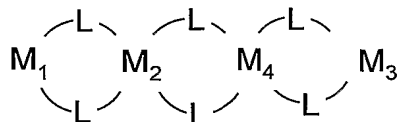
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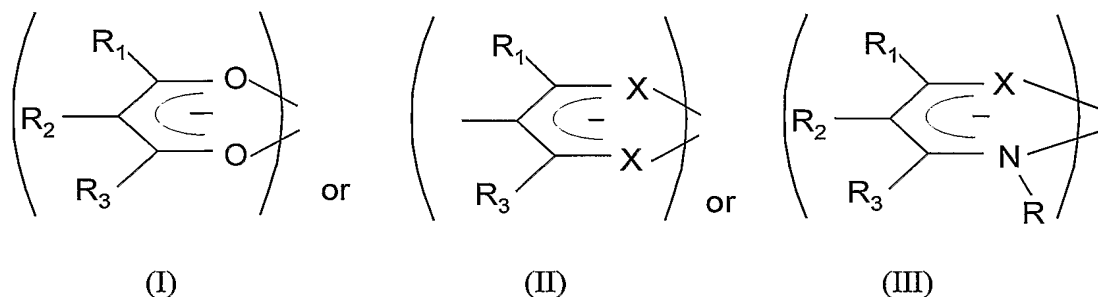
- 8 -



where  $M_1$ ,  $M_2$ ,  $M_3$  and  $M_4$  are rare earth metals and L is a bridging ligand.

- 5 The metal  $M_2$  can be any metal which is not a rare earth, transition metal, lanthanide or an actinide examples of metals which can be used include lithium, sodium, potassium, rubidium, caesium, beryllium, magnesium, calcium, strontium, barium, copper, silver, gold, zinc, cadmium, boron, aluminium, gallium, indium, germanium, tin, antimony, lead, and metals of the first, second and third groups of transition metals e.g. manganese, iron, ruthenium, osmium, cobalt, nickel, palladium, platinum,
- 10 cadmium, chromium. titanium, vanadium, zirconium, tantalum, molybdenum, rhodium, iridium, titanium, niobium, scandium, yttrium etc.

Preferably  $L\alpha$  is selected from  $\beta$  diketones such as those of formulae



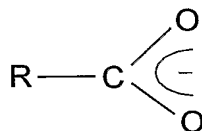
- 15 where  $R_1$ ,  $R_2$  and  $R_3$  can be the same or different and are selected from hydrogen, and substituted and unsubstituted hydrocarbyl groups such as substituted and unsubstituted aliphatic groups, substituted and unsubstituted aromatic, heterocyclic and polycyclic ring structures, fluorocarbons such as trifluoromethyl groups,
- 20 halogens such as fluorine or thiophenyl groups;  $R_1$ ,  $R_2$  and  $R_3$  can also form substituted and unsubstituted fused aromatic, heterocyclic and polycyclic ring structures and can be copolymerisable with a monomer e.g. styrene. X is Se, S or O, Y can be hydrogen, substituted or unsubstituted hydrocarbyl groups, such as substituted and unsubstituted aromatic, heterocyclic and polycyclic ring structures,

- 9 -

fluorine, fluorocarbons such as trifluoromethyl groups, halogens such as fluorine or thiophenyl groups or nitrile.

- 5 Examples of  $R_1$  and/or  $R_2$  and/or  $R_3$  include aliphatic, aromatic and heterocyclic alkoxy, aryloxy and carboxy groups, substituted and substituted phenyl, fluorophenyl, biphenyl, phenanthrene, anthracene, naphthyl and fluorene groups alkyl groups such as t-butyl, heterocyclic groups such as carbazole.

- 10 Some of the different groups  $L_\alpha$  may also be the same or different charged groups such as carboxylate groups so that the group  $L_1$  can be as defined above and the groups  $L_2, L_3...$  can be charged groups such as



(IV)

- 15 where R is  $R_1$  as defined above or the groups  $L_1, L_2$  can be as defined above and  $L_3...$  etc. are other charged groups.

$R_1, R_2$  and  $R_3$  can also be



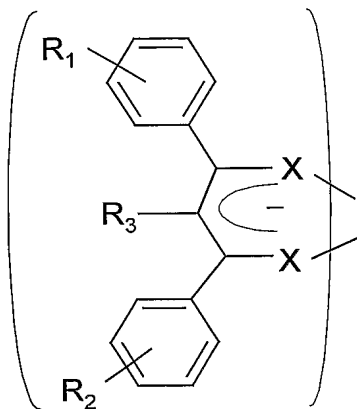
where X is O, S, Se or NH.

(V)

- 20 A preferred moiety  $R_1$  is trifluoromethyl  $\text{CF}_3$  and examples of such diketones are, benzoyltrifluoroacetone, p-chlorobenzoyltrifluoroacetone, p-bromotrifluoroacetone, p-phenyltrifluoroacetone, 1-naphthoyltrifluoroacetone, 2-naphthoyltrifluoroacetone, 2-phenathoyltrifluoroacetone, 3-phenanthoyltrifluoroacetone, 9-anthroyltrifluoroacetone, trifluoroacetone, cinnamoyltrifluoroacetone, and 2-thenoyltrifluoroacetone.
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The different groups  $L\alpha$  may be the same or different ligands of formulae

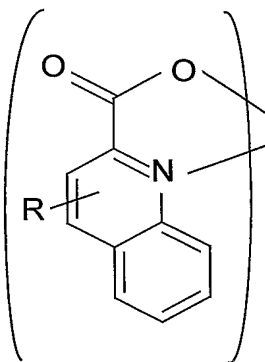


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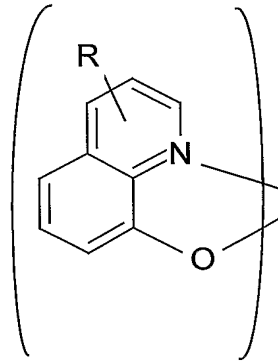
where X is O, S, or Se and  $R_1$ ,  $R_2$  and  $R_3$  are as above.

The different groups  $L\alpha$  may be the same or different quinolate derivatives such as



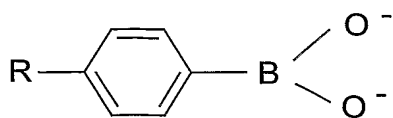
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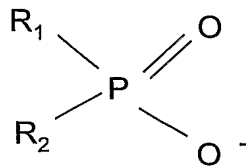
(VIII)

10 where R is hydrocarbyl, aliphatic, aromatic or heterocyclic carboxy, aryloxy, hydroxy or alkoxy e.g. the 8 hydroxy quinolate derivatives or



(IX)

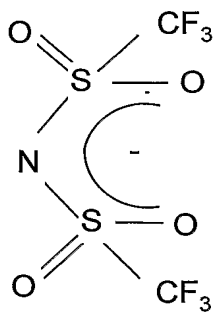
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(X)

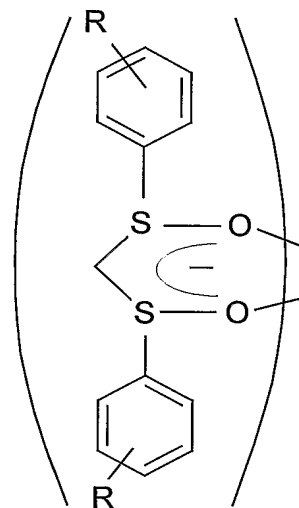
- 11 -

where R, R<sub>1</sub>, and R<sub>2</sub> are as above or are H or F e.g. R<sub>1</sub> and R<sub>2</sub> are alkyl or alkoxy groups



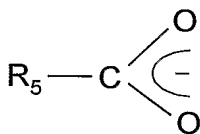
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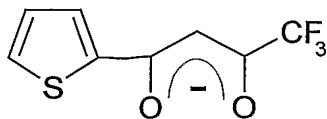
(XII)

- 5 As stated above the different groups L<sub>α</sub> may also be the same or different carboxylate groups e.g.

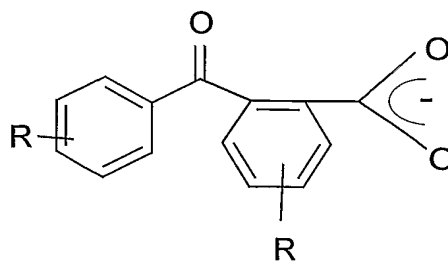


(XIII)

- where R<sub>5</sub> is a substituted or unsubstituted aromatic, polycyclic or heterocyclic ring a polypyridyl group, R<sub>5</sub> can also be a 2-ethyl hexyl group so L<sub>n</sub> is 2-ethylhexanoate or R<sub>5</sub> can be a chair structure so that L<sub>n</sub> is 2-acetyl cyclohexanoate or L<sub>α</sub> can be
- 10



(XIV)

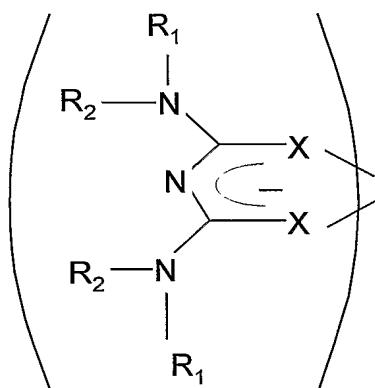


(XIVa)

- 12 -

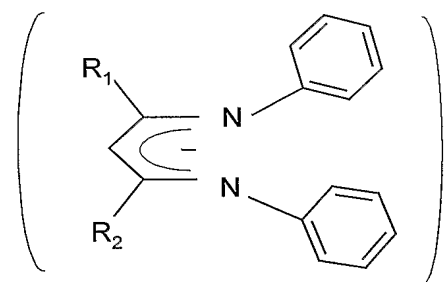
where R is as above e.g. alkyl, allenyl, amino or a fused ring such as a cyclic or polycyclic ring.

5 The different groups  $L\alpha$  may also be



(XV)

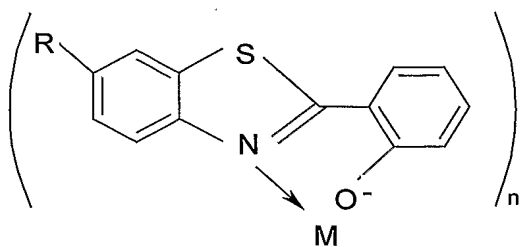
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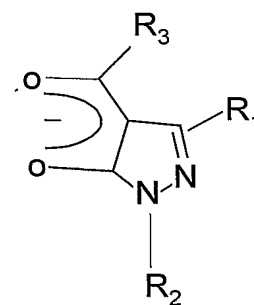
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(XVII)

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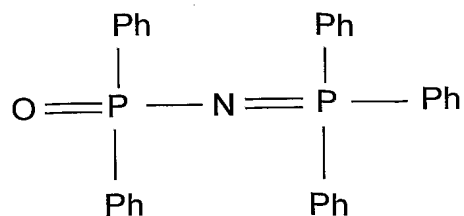
(XVIIa)

Where R,  $R_1$  and  $R_2$  are as above.

15

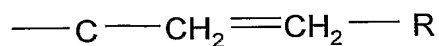
The groups  $L_p$  can be selected from

- 13 -



(XVIII)

where each Ph which can be the same or different and can be a phenyl (OPNP) or a  
 5 substituted phenyl group, other substituted or unsubstituted aromatic group, a  
 substituted or unsubstituted heterocyclic or polycyclic group, a substituted or  
 unsubstituted fused aromatic group such as a naphthyl, anthracene, phenanthrene or  
 pyrene group. The substituents can be for example an alkyl, aralkyl, alkoxy, aromatic,  
 heterocyclic, polycyclic group, halogen such as fluorine, cyano, amino. Substituted  
 10 amino etc. Examples are given in figs. 1 and 2 of the drawings where R, R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub>  
 and R<sub>4</sub> can be the same or different and are selected from hydrogen, hydrocarbyl  
 groups, substituted and unsubstituted aromatic, heterocyclic and polycyclic ring  
 structures, fluorocarbons such as trifluoryl methyl groups, halogens such as fluorine  
 or thiophenyl groups; R, R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> and R<sub>4</sub> can also form substituted and unsubstituted  
 15 fused aromatic, heterocyclic and polycyclic ring structures and can be  
 copolymerisable with a monomer e.g. styrene. R, R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> and R<sub>4</sub> can also be  
 unsaturated alkylene groups such as vinyl groups or groups

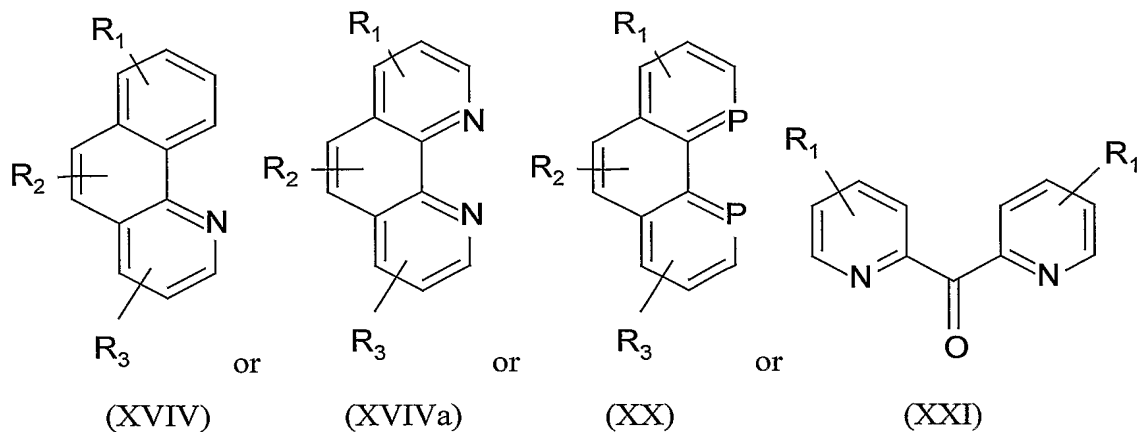


where R is as above.

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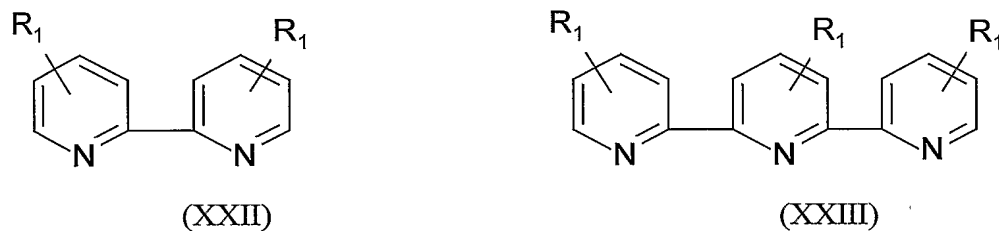
L<sub>p</sub> can also be compounds of formulae

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where  $R_1$ ,  $R_2$  and  $R_3$  are as referred to above, for example bathophen shown in fig. 3 of the drawings in which R is as above or

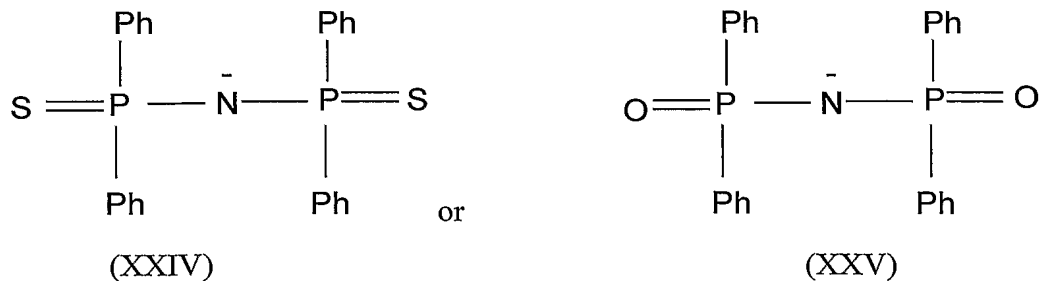
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where  $R_1$ ,  $R_2$  and  $R_3$  are as referred to above.

10

$L_p$  can also be



15

where Ph is as above.

- 15 -

Other examples of  $L_p$  chelates are as shown in figs. 4 and fluorene and fluorene derivatives e.g. a shown in figs. 5 and compounds of formulae as shown as shown in figs. 6 to 8.

- 5 Specific examples of  $L_\alpha$  and  $L_p$  are tripyridyl and TMHD, and TMHD complexes,  $\alpha$ ,  $\alpha'$ ,  $\alpha''$  tripyridyl, crown ethers, cyclans, cryptans phthalocyanans, porphoryins ethylene diamine tetramine (EDTA), DCTA, DTPA and TTHA, where TMHD is 2,2,6,6-tetramethyl-3,5-heptanedionato and OPNP is diphenylphosphonimide triphenyl phosphorane. The formulae of the polyamines are shown in fig. 9.

10

Other electroluminescent materials which can be used include metal quinolates such as lithium quinolate, aluminium quinolate, scandium quinolate zirconium quinolate, hafnium quinolate vanadium quinolate etc. The quinolates can be doped e.g. with a dye such as diphenylquinacridine, diphenylquinacridone, coumarins, perylene and their derivatives.

15

- Other electroluminescent materials which can be used include organic complexes of non rare earth metals such as lithium, sodium, potassium, rubidium, caesium, beryllium, magnesium, calcium, strontium, barium, copper, silver, gold, zinc, cadmium, boron, aluminium, gallium, indium, germanium, tin, antimony, lead, and metals of the first, second and third groups of transition metals e.g. manganese, iron, ruthenium, osmium, cobalt, nickel, palladium, platinum, cadmium, chromium, titanium, vanadium, zirconium, tantalum, molybdenum, rhodium, iridium, titanium, niobium, scandium, yttrium etc. which emit light when an electric current is passed through it. The complexes can be formed with the ligands of formula (I) to (XVII) above, optionally with a neutral ligand of formula  $L_p$  as defined above.

25

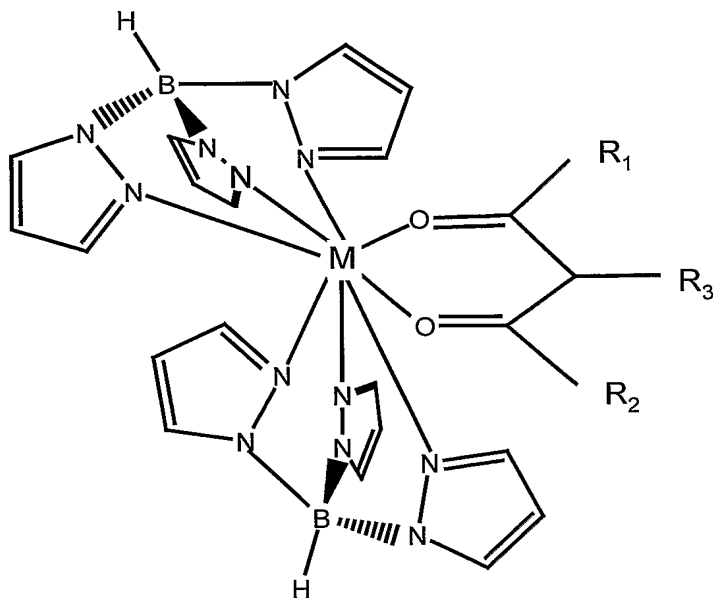
- Such complexes are complexes of  $\beta$ -diketones e.g. tris -(1,3-diphenyl-1,3-propanedione) (DBM) and suitable metal complexes are  $Al(DBM)_3$ ,  $Zn(DBM)_2$  and  $Mg(DBM)_2$ ,  $Sc(DBM)_3$  etc.

30



- 16 -

Further complexes which can be used as the photovoltaic element are borate complexes of formula



where M is a rare earth, lanthanide or an actinide and R<sub>1</sub>, R<sub>2</sub> and R<sub>3</sub> are as defined above.

A photovoltaic device can be made in the conventional way for example by forming a layer of the metal chelate on a metal so the metal forms a first electrode and preferably the other, second electrode, comprises a transparent conductive layer. This electrode is preferably a transparent substrate which is a conductive glass or plastic material which acts as the cathode; preferred substrates are conductive glasses such as indium tin oxide coated glass, but any glass which is conductive or has a conductive layer can be used, so that, when light falls on the metal chelate an electric field is generated between the electrodes.

15

There are a very large number of designs for photovoltaic devices and solar cells and a survey of such devices is given in the Jean-Michel Nunzi Article referred to above and in the references thereto. In general the metal chelates can be used as the photovoltaic element in such devices.

- 17 -

The metal chelate material can be deposited on the metal or conductive transparent material substrate directly by evaporation from a solution of the material in an organic solvent. The solvent which is used will depend on the material, but  
5 chlorinated hydrocarbons such as dichloromethane, n-methyl pyrrolidone, dimethyl sulphoxide, tetra hydrofuran dimethylformamide etc. are suitable in many cases.

Alternatively the material can be deposited by spin coating from solution or by vacuum deposition from the solid state e.g. by sputtering or any other conventional  
10 method can be used.

As stated above, the electrons by absorption of solar radiation of the appropriate bandgap, produce electron-hole pairs. The separation of the electron-hole pairs with the electrons flowing toward the region of N-type conductivity, and the holes flowing  
15 toward the region of P-type conductivity, creates the photovoltage and photocurrent of the cell. By having a layer of a hole transmitting material, i.e. a p-type transmitter between the cathode and the metal chelate and/or a layer of an electron transmitting material between the metal chelate and the anode, increased mobility of the holes and the electrons can be achieved increasing the effectiveness of the photovoltaic cell.

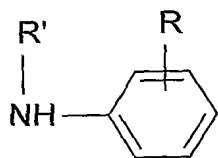
20

Hole transmitting layers are used in polymer electroluminescent devices and any of the known hole transmitting materials in film form can be used.

The hole transporting material can be an amine complex such as poly  
25 (vinylcarbazole), N, N'-diphenyl-N, N'-bis (3-methylphenyl) -1,1' -biphenyl -4,4'-diamine (TPD), an unsubstituted or substituted polymer of an amino substituted aromatic compound, a polyaniline, substituted polyanilines, polythiophenes, substituted polythiophenes, polysilanes etc. Examples of polyanilines are polymers of

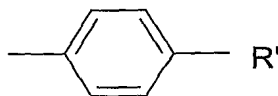
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- 18 -



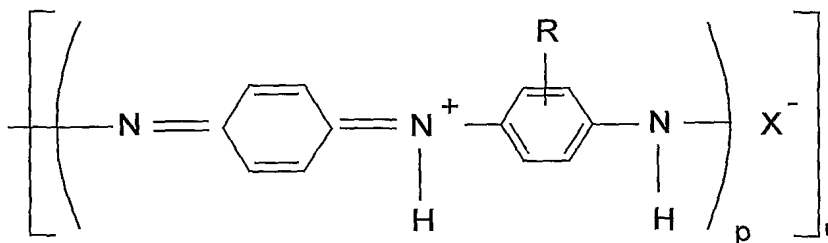
(XXVI)

- 5 where R is in the ortho – or meta-position and is hydrogen, C1-18 alkyl, C1-6 alkoxy, amino, chloro, bromo, hydroxy or the group



- 10 where R is alkyl or aryl and R' is hydrogen, C1-6 alkyl or aryl with at least one other monomer of formula I above.

Or the hole transporting material can be a polyaniline. Polyanilines which can be used in the present invention have the general formula



(XXVII)

- 15 where p is from 1 to 10 and n is from 1 to 20, R is as defined above and X is an anion, preferably selected from Cl, Br, SO<sub>4</sub>, BF<sub>4</sub>, PF<sub>6</sub>, H<sub>2</sub>PO<sub>3</sub>, H<sub>2</sub>PO<sub>4</sub>, arylsulphonate, arenedicarboxylate, polystyrenesulphonate, polyacrylate
- 20 alkylsulphonate, vinylsulphonate, vinylbenzene sulphonate, cellulose sulphonate, camphor sulphonates, cellulose sulphate or a perfluorinated polyanion.

- 19 -

Examples of arylsulphonates are p-toluenesulphonate, benzenesulphonate, 9,10-anthraquinone-sulphonate and anthracenesulphonate; an example of an arenedicarboxylate is phthalate and an example of arenecarboxylate is benzoate.

5

We have found that protonated polymers of the unsubstituted or substituted polymer of an amino substituted aromatic compound such as a polyaniline are difficult to evaporate or cannot be evaporated, however we have surprisingly found that if the unsubstituted or substituted polymer of an amino substituted aromatic compound is

10 deprotonated then it can be easily evaporated i.e. the polymer is evaporable.

Preferably evaporable deprotonated polymers of unsubstituted or substituted polymer of an amino substituted aromatic compound are used. The de-protonated unsubstituted or substituted polymer of an amino substituted aromatic compound can

15 be formed by deprotonating the polymer by treatment with an alkali such as ammonium hydroxide or an alkali metal hydroxide such as sodium hydroxide or potassium hydroxide.

The degree of protonation can be controlled by forming a protonated polyaniline and

20 de-protonating. Methods of preparing polyanilines are described in the article by A. G. MacDiarmid and A. F. Epstein, Faraday Discussions, Chem Soc.88 P319 1989.

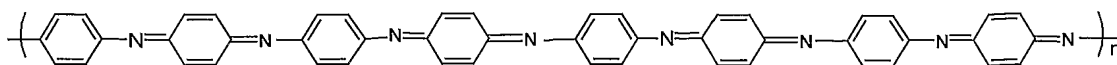
The conductivity of the polyaniline is dependant on the degree of protonation with the maximum conductivity being when the degree of protonation is between 40 and 60%

25 e.g. about 50%.

Preferably the polymer is substantially fully deprotonated.

A polyaniline can be formed of octamer units i.e. p is four e.g.

- 20 -



The polyanilines can have conductivities of the order of  $1 \times 10^{-1}$  Siemen  $\text{cm}^{-1}$  or higher.

5

The aromatic rings can be unsubstituted or substituted e.g. by a C1 to 20 alkyl group such as ethyl.

10

The polyaniline can be a copolymer of aniline and preferred copolymers are the copolymers of aniline with o-anisidine, m-sulphanilic acid or o-aminophenol, or o-toluidine with o-aminophenol, o-ethylaniline, o-phenylene diamine or with amino anthracenes.

15

Other polymers of an amino substituted aromatic compound which can be used include substituted or unsubstituted polyaminonaphthalenes, polyaminoanthracenes, polyaminophenanthrenes, etc. and polymers of any other condensed polyaromatic compound. Polyaminoanthracenes and methods of making them are disclosed in US Patent 6,153,726. The aromatic rings can be unsubstituted or substituted e.g. by a group R as defined above.

20

Other hole transporting materials are conjugated polymer and the conjugated polymers which can be used can be any of the conjugated polymers disclosed or referred to in US 5807627, PCT/WO90/13148 and PCT/WO92/03490.

25

The preferred conjugated polymers are poly (p-phenylenevinylene)-PPV and copolymers including PPV. Other preferred polymers are poly(2,5 dialkoxyphenylene vinylene) such as poly (2-methoxy-5-(2-methoxypentyloxy)-1,4-phenylene vinylene), poly(2-methoxypentyloxy)-1,4-phenylenevinylene), poly(2-methoxy-5-(2-dodecyloxy)-1,4-phenylenevinylene) and other poly(2,5 dialkoxyphenylenevinylens)

- 21 -

with at least one of the alkoxy groups being a long chain solubilising alkoxy group, polyfluorenes and oligofluorenes, polyphenylenes and oligophenylenes, polyanthracenes and oligo anthracenes, ploythiophenes and oligothiophenes.

- 5 In PPV the phenylene ring may optionally carry one or more substituents e.g. each independently selected from alkyl, preferably methyl, alkoxy, preferably methoxy or ethoxy.

- Any poly(arylenevinylene) including substituted derivatives thereof can be used and  
10 the phenylene ring in poly(p-phenylenevinylene) may be replaced by a fused ring system such as anthracene or naphthylene ring and the number of vinylene groups in each polyphenylenevinylene moiety can be increased e.g. up to 7 or higher.

- The conjugated polymers can be made by the methods disclosed in US 5807627,  
15 PCT/WO90/13148 and PCT/WO92/03490.

The thickness of the hole transporting layer is preferably 20nm to 200nm.

- The polymers of an amino substituted aromatic compound such as polyanilines  
20 referred to above can also be used as buffer layers with or in conjunction with other hole transporting materials.

- The structural formulae of some other hole transporting materials are shown in  
Figures 12, 13, 14, 15 and 16 of the drawings, where R<sub>1</sub>, R<sub>2</sub> and R<sub>3</sub> can be the same or  
25 different and are selected from hydrogen, and substituted and unsubstituted hydrocarbyl groups such as substituted and unsubstituted aliphatic groups, substituted and unsubstituted aromatic, heterocyclic and polycyclic ring structures, fluorocarbons such as trifluoromethyl groups, halogens such as fluorine or thiophenyl groups; R<sub>1</sub>, R<sub>2</sub> and R<sub>3</sub> can also form substituted and unsubstituted fused aromatic, heterocyclic  
30 and polycyclic ring structures and can be copolymerisable with a monomer e.g.

- 22 -

styrene. X is Se, S or O, Y can be hydrogen, substituted or unsubstituted hydrocarbyl groups, such as substituted and unsubstituted aromatic, heterocyclic and polycyclic ring structures, fluorine, fluorocarbons such as trifluoromethyl groups, halogens such as fluorine or thiophenyl groups or nitrile.

5

Examples of R<sub>1</sub> and/or R<sub>2</sub> and/or R<sub>3</sub> include aliphatic, aromatic and heterocyclic alkoxy, aryloxy and carboxy groups, substituted and unsubstituted phenyl, fluorophenyl, biphenyl, phenanthrene, anthracene, naphthyl and fluorene groups alkyl groups such as t-butyl, heterocyclic groups such as carbazole.

10

Optionally there is a layer of an electron injecting material between the anode and the electroluminescent material layer; the electron injecting material is a material which will transport electrons when an electric current is passed through it; electron injecting materials include a metal complex such as a metal quinolate e.g. an aluminium quinolate, lithium quinolate, a cyano anthracene such as 9,10 dicyano anthracene, cyano substituted aromatic compounds, tetracyanoquinodimethane a polystyrene sulphonate or a compound with the structural formulae shown in figures 9 or 10 of the drawings in which the phenyl rings can be substituted with substituents R as defined above.

15

20

The cathode is preferably a transparent substrate such as a conductive glass or plastic material which acts as the anode. Preferred substrates are conductive glasses such as indium tin oxide coated glass, but any glass which is conductive or has a conductive layer such as a metal or conductive polymer can be used. Conductive polymers and conductive polymer coated glass or plastics materials can also be used as the substrate.

25

The anode is preferably a low work function metal e.g. aluminium, calcium, lithium, silver/magnesium alloys, rare earth metal alloys etc., aluminium is a preferred metal.

- 23 -

A metal fluoride such as an alkali metal, rare earth metal or their alloys can be used as the second electrode for example by having a metal fluoride layer formed on a metal.

- 5 As stated above, the photocurrent output of a solar cell is maximized by increasing the total number of photons of differing energy and wavelength which are absorbed by the semiconductor material and it is a feature of the present invention that the rare earth metal chelates can absorb light of a specific wavelength depending on the metal and ligands used so, by having a plurality of layers of different metal chelates of
- 10 differing bandgaps which absorb light at different wavelengths, a wide range of the visible spectrum can be used. Metal chelates can be also used which will absorb light in the infra-red, ultra-violet or shorter wavelengths so improving the utilisation of sunlight and increasing the power achievable by a solar cell.
- 15 As stated above, the photocurrent output of a solar cell is maximized by increasing the total number of photons of differing energy and wavelength which are absorbed by the semiconductor material and it is a feature of the present invention that the rare earth metal chelates can absorb light of a specific wavelength depending on the metal and ligands used so, by having a plurality of layers of different metal chelates of
- 20 differing bandgaps which absorb light at different wavelengths, a wide range of the visible spectrum can be used. Metal chelates can be also used which will absorb light in the infra-red, ultra-violet or shorter wavelengths so improving the utilisation of sunlight and increasing the power achievable by a solar cell.
- 25 Alternatively individual solar cells of differing bandgap energies i.e. using different metal chelates of differing bandgaps which absorb light at different wavelengths can be connected in series.

Devices of the invention are illustrated in the drawings in which:-



Fig. 17 shows a simple photovoltaic cell

Figs. 18 and 19 show other cells and

Fig. 20 shows a tandem cell

5

Referring to fig. 17 a simple cell comprises a metal anode e.g. made of aluminium (1) a layer of an electroluminescent material (2) as described herein and a cathode comprising an indium titanium oxide (ITO) coated glass (3). When light passes through the ITO coated glass it is absorbed by the electroluminescent material layer (2), which is the photovoltaic element, and an electric field is generated between the anode and cathode and when the anode and cathode are connected through an electric circuit an electric current will flow between them.

10

Referring to fig. 18 there is a layer of an electron transmitting material (4) between the layers (2) and (1).

15

Referring to fig. 19 there is a layer of a hole transporting layer (5) between the layers (2) and (3).

Referring to fig. 20 this shows a tandem solar cell in which there are a plurality of cells in series of fig. 17 formed of a cathode (11), an electroluminescent layer (13) and anode (12) so that a larger field is generated between the end anode and cathode, in order for there to be a transmission of light through the cells the anodes and cathodes of the intermediate cells are transparent. At least some of the photovoltaic elements (13) in each of the cells are different to adsorb light at a range of wavelengths.

20

25

#### Example 1

A photovoltaic device was fabricated on a clean and dried ITO coated glass piece (1 x 1 cm<sup>2</sup>) by sequentially forming layers by vacuum evaporation to form a structure

30

- 25 -

ITO/CuPc(20nm)/TPD(50nm)/ Eu (DBM)<sub>3</sub>(OPNP)/(85nm)Alq<sub>3</sub>/LiF(0.4nm)/Al

Where CuPc is copper phthalocyanine, TPD is N, N'-diphenyl-N, N'-bis (3-methylphenyl) -1,1' -biphenyl -4,4'-diamine, Alq<sub>3</sub> is aluminium quinolate, LiF is lithium fluoride and Al is aluminium.

To deposit the layers the organic coating on the portion which had been etched with the concentrated hydrochloric acid was wiped with a cotton bud. The coated electrodes were stored in a vacuum desiccator over a molecular sieve and phosphorous pentoxide until they were loaded into a vacuum coater (Edwards, 10<sup>-6</sup> torr) and aluminium top contacts made. The active area of the photovoltaic device was 0.08 cm by 0.1 cm<sup>2</sup> the devices were then kept in a vacuum desiccator until the photovoltaic studies were performed.

The device was connected in an electric circuit and exposed to light of various wavelengths  $\lambda$  and the voltage and current measured the results are shown graphically in fig. 21 where the open circuit voltage Voc and short circuit current Jsc (as described in the Jean-Michel Nunzi Article referred to above) were obtained. The white light was obtained from a simulated daylight fluorescent bulb.

#### Example 2

Example 1 was repeated using a structure comprising

ITO/CuPc(20nm)/ $\alpha$ -NPB(75nm)/Zr<sub>q4</sub>:DPQA(75:0.75nm)/Zr<sub>q4</sub>10nm)Alq<sub>3</sub>/LiF(0.4nm)/Al

Where  $\alpha$ -NPB is as shown in fig. 16a, DPQA is diphenylquinacridone.

- 26 -

The Zrq<sub>4</sub> is zirconium quinolate and the Zrq<sub>4</sub>:DPQA layer was formed by concurrent vacuum deposition to form a zirconium quinolate layer doped with DPQA. The weight ratio of the Zrq<sub>4</sub> and DPQA is conveniently shown by a relative thickness measurement.

5

The device was connected in an electric circuit and exposed to light of various wavelengths  $\lambda$  and the voltage and current measured the results are shown graphically in fig. 22 where the open circuit voltage Voc and short circuit current Jsc (as described in the Jean-Michel Nunzi Article referred to above) were obtained. The

10

white light was obtained from a simulated daylight fluorescent bulb.

### Example 3

Example 1 was repeated using a structure comprising

15

ITO/CuPc(20nm)/ $\alpha$ -NPB(75nm)/Liq(65nm)/Al.

Where Liq is lithium quinolate

20

The device was connected in an electric circuit and exposed to light of various wavelengths  $\lambda$  and the voltage and current measured the results are shown graphically in fig. 23 where the open circuit voltage Voc and short circuit current Jsc (as described in the Jean-Michel Nunzi Article referred to above) were obtained. The white light was obtained from a simulated daylight fluorescent bulb.

25

### Example 4

Example 1 was repeated using a structure comprising

- 27 -

ITO/CuPc(20nm)/ $\alpha$ -NPB(75nm)/Liq(65nm)LiF(0.4nm)/Al.

The device was connected in an electric circuit and exposed to light of various wavelengths  $\lambda$  and the voltage and current measured the results are shown graphically in fig. 24 where the open circuit voltage  $V_{oc}$  and short circuit current  $J_{sc}$  (as described in the Jean-Michel Nunzi Article referred to above) were obtained. The white light was obtained from a simulated daylight fluorescent bulb.

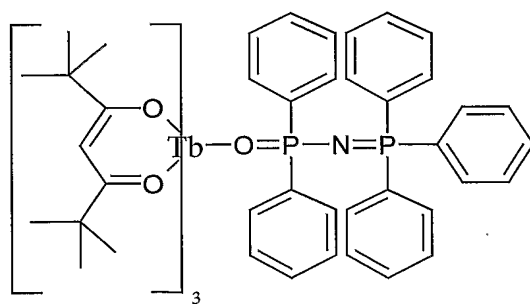
#### Example 5

Devices were made as in Example 1 of structure

ITO/CuPc(25)/ $\alpha$ -NPB(80)/CBP:Compound A(30:2)/BCP(10)/Zr<sub>q</sub>4(60)/LiF(0.2)/Al

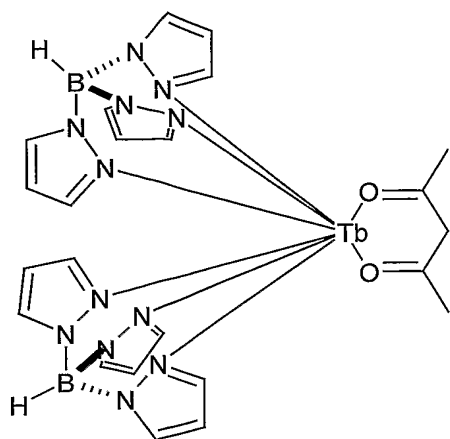
Where the film thicknesses are in nanometres and CBP is as in fig. 4b and BCP is bathocupron

compound A was

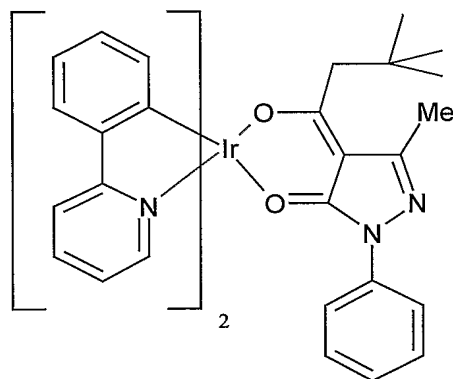


Similar devices were made with compounds B and C in place of compound A where compound B is

- 28 -



and compound C is



5

The results are shown in the Table

Table

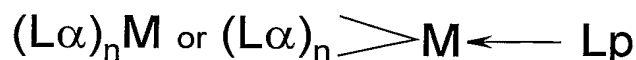
Photovoltaic element	$V_{\text{Ph}}^{\text{OC}} / \text{mV}$	$J_{\text{Ph}}^{\text{SC}} / \text{mA cm}^{-2}$	$\lambda / \text{nm}$
A	7.5	- 0.4	600
B	-0.3	2.2	500
C	-159	0.4	550

10

- 29 -

## Claims

1. A photovoltaic device comprising a metal chelate as the photovoltaic element.
- 5 2. A photovoltaic device as claimed in claim 1 which comprises sequentially (i) a first electrode comprising a metal, (ii) the photovoltaic element and (iii) a second electrode.
3. A device as claimed in claim 1 or 2 in which the photovoltaic element comprises
- 10 an organo metallic complex of formula



- where L $\alpha$  and Lp are organic ligands, M is a metal and n is the valence state of the
- 15 metal M and in which the ligands L $\alpha$  are the same or different.

4. A device as claimed in any one of claims 1 to 4 in which the metal M is a rare earth, transition metal, lanthanide or an actinide.
- 20 5. A device as claimed in claim 4 in which the said rare earth, transition metal, lanthanide or an actinide is selected from Sm(III), Eu(II), Eu(III), Tb(III), Dy(III), Yb(III), Lu(III), Gd (III), Gd(III) U(III), Tm(III), Ce (III), Pr(III), Nd(III), Pm(III), Dy(III), Ho(III) and Er(III).
- 25 6. A device as claimed in any one of claims 1 to 3 in which the metal M is a non rare earth metal.
7. A device as claimed in claim 6 in which the metal M is selected from lithium, sodium, potassium, rubidium, caesium, beryllium, magnesium, calcium, strontium,

- 30 -

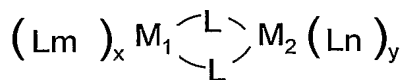
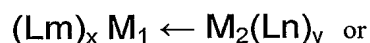
barium, copper, silver, gold, zinc, cadmium, boron, aluminium, gallium, indium, germanium, tin, antimony, lead, and metals of the first, second and third groups of transition metals, manganese, iron, ruthenium, osmium, cobalt, nickel, palladium, platinum, cadmium, chromium. titanium, vanadium, zirconium, tantalum,  
 5 molybdenum, rhodium, iridium, titanium, niobium, scandium and yttrium.

8. A device as claimed in any one of claims 3 to 7 in which there are a plurality of ligands  $L_p$  which can be the same or different.

10 9. A device as claimed in any one of the preceding claims in which the photovoltaic element comprises an organo metallic complex of formula  $(L_n)_n M_1 M_2$  or  $(L_n)_n M_1 M_2 (L_p)$ , where  $L_n$  is  $L_\alpha$ ,  $L_p$  is a neutral ligand  $M_1$  is a rare earth, transition metal, lanthanide or an actinide,  $M_2$  is a non rare earth metal and  $n$  is the combined valence state of  $M_1$  and  $M_2$ .

15

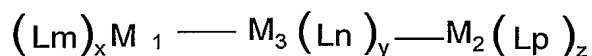
10. A device as claimed in any one of the preceding claims in which the photovoltaic element comprises a binuclear, trinuclear or polynuclear organometallic complex of formula



20

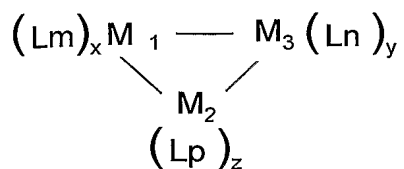
where  $L$  is a bridging ligand and where  $M_1$  is a rare earth metal and  $M_2$  is  $M_1$  or a non rare earth metal,  $L_m$  and  $L_n$  are the same or different organic ligands  $L_\alpha$  as defined above,  $x$  is the valence state of  $M_1$  and  $y$  is the valence state of  $M_2$  or

25

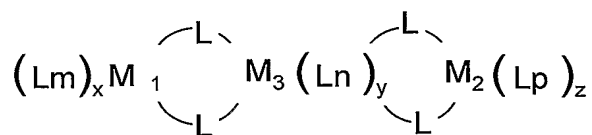


or

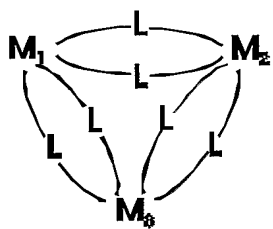
- 31 -



- 5 where  $\text{M}_1$ ,  $\text{M}_2$  and  $\text{M}_3$  are the same or different rare earth metals and Lm, Ln and Lp are organic ligands La and x is the valence state of  $\text{M}_1$ , y is the valence state of  $\text{M}_2$  and z is the valence state of  $\text{M}_3$  and Lp can be the same as Lm and Ln or different or

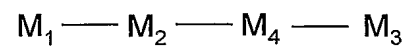


10 or



or

15  $\text{M}_1 \text{ --- } \text{M}_2 \text{ --- } \text{M}_3 \text{ --- } \text{M}_4$   
or

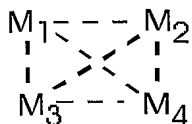


or

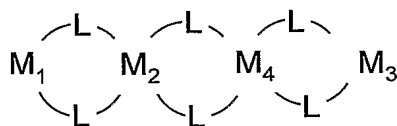
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- 32 -



or



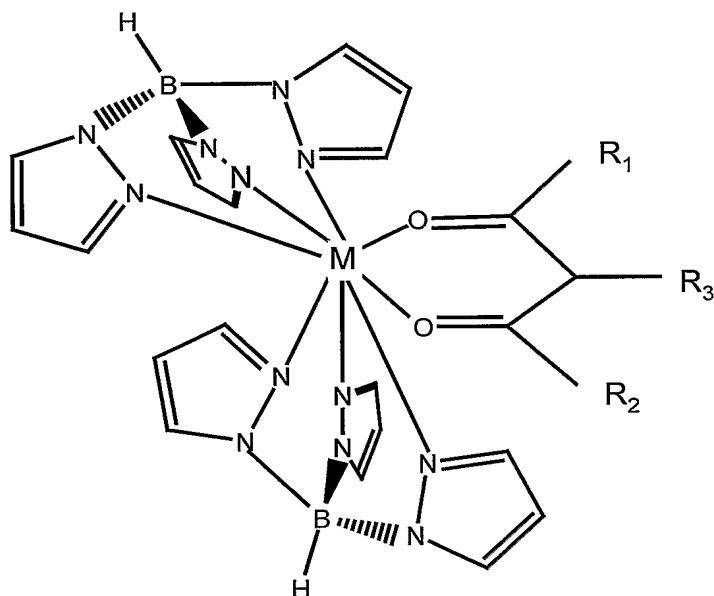
- 5 where  $M_4$  is  $M_1$  and L is a bridging ligand and in which the rare earth metals and the non rare earth metals can be joined together by a metal to metal bond and/or via an intermediate bridging atom, ligand or molecular group or in which there are more than three metals joined by metal to metal bonds and/or via intermediate ligands and
- 10 11. A device as claimed in any one of claims 3 to 10 in which  $L\alpha$  has the formula (I) to (XVII) herein.
12. A device as claimed in any one of claims 3 to 11 in which  $Lp$  has the formula of figs. 1 to 8 of the accompanying drawings or of formula (XVIII) to (XXV) herein.
- 15 13. A device as claimed in claim 1 or 2 in which the organometallic chelate is a metal quinolate.
14. A device as claimed in claim 13 in which the metal quinolate is lithium quinolate,
- 20 aluminium quinolate, scandium quinolate zirconium quinolate, hafnium quinolate or vanadium quinolate.
15. A device as claimed in claim 14 in which the metal quinolate is doped with a fluorescent, phosphorescence or ion fluorescent compound.

25

- 33 -

16. A device as claimed in claim 15 in which the dopant is diphenylquinacridine, diphenylquinacridone, coumarins, perylene or their derivatives.

17. A device as claimed in claim 1 or 2 in which the photovoltaic element has the  
5 formula



where M is a rare earth, transition metal, lanthanide or an actinide and R<sub>1</sub>, R<sub>2</sub> and R<sub>3</sub>  
10 can be the same or different and are selected from hydrogen, and substituted and unsubstituted hydrocarbyl groups, substituted and unsubstituted aliphatic groups, substituted and unsubstituted aromatic, heterocyclic and polycyclic ring structures, fluorocarbons and trifluoromethyl groups, halogens and thiophenyl groups.

15 18. A device as claimed in any one of claims 2 to 17 in which the second electrode comprises a transparent substrate which is a conductive glass or plastic material and which covers at least part of the photovoltaic element.

- 34 -

19. A device as claimed in any one of the preceding claims which comprises sequentially (i) a first electrode comprising a metal, (ii) a plurality of layers of photovoltaic elements in which the photovoltaic elements in at least two of the layers are different and (iii) a second electrode.

5

20. A device as claimed in claim 19 in which at least some of the different photovoltaic elements absorb light at different wavelengths.

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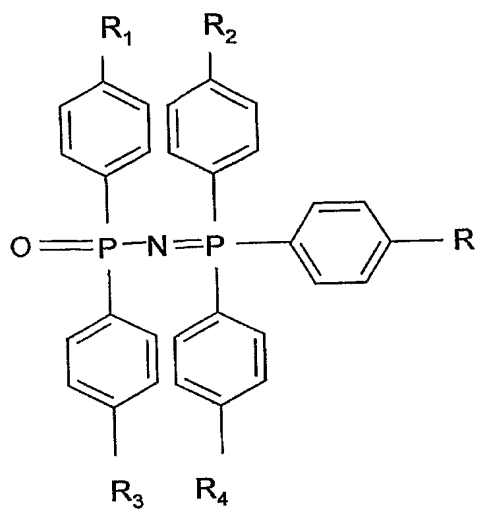


Fig. 1

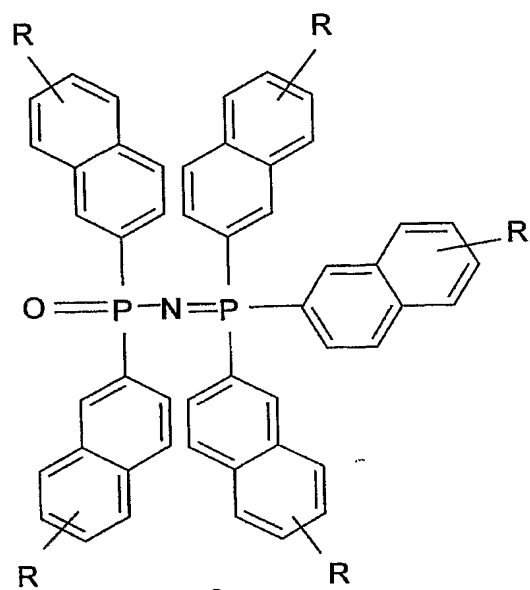


Fig. 2a

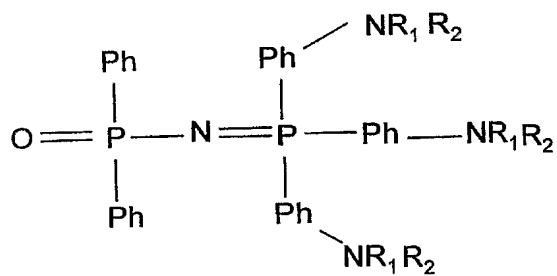


Fig. 2b

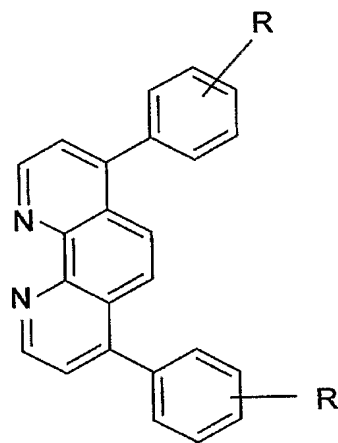


Fig. 3

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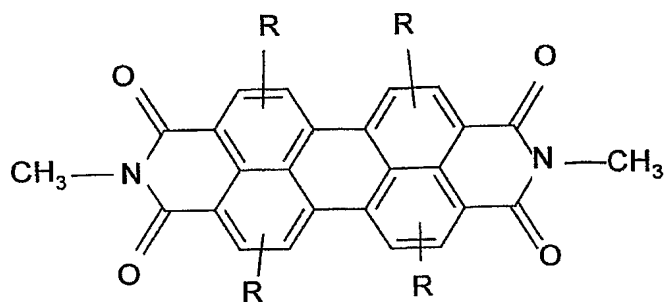


Fig. 4a

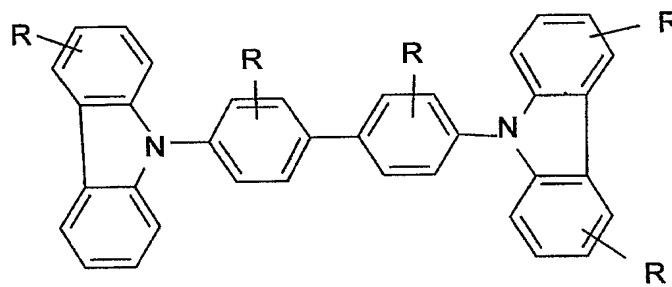


Fig. 4b

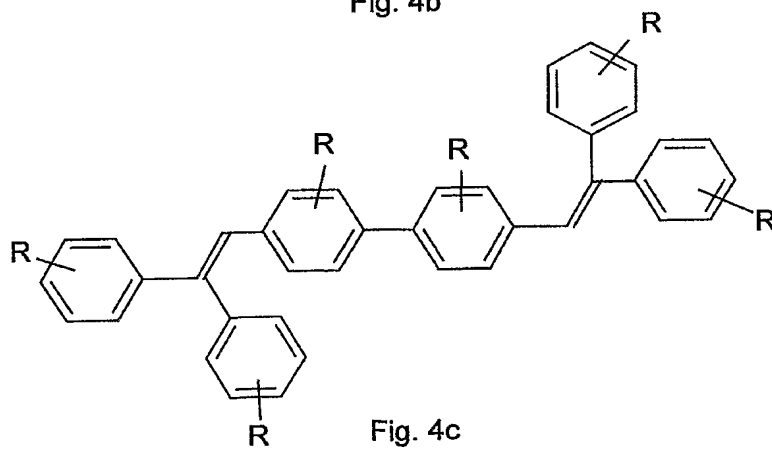


Fig. 4c

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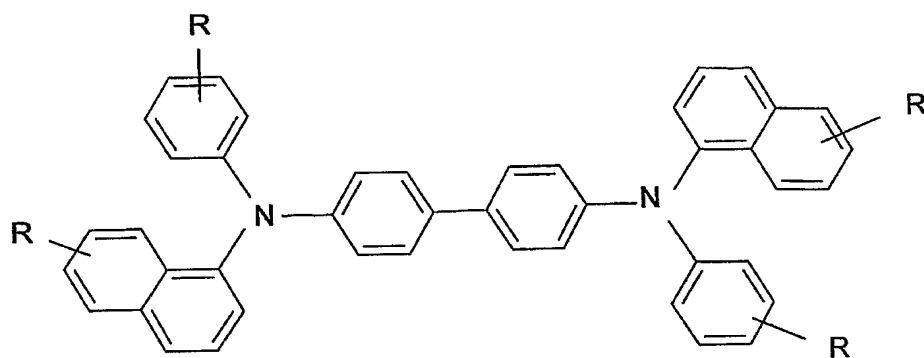


Fig. 4d

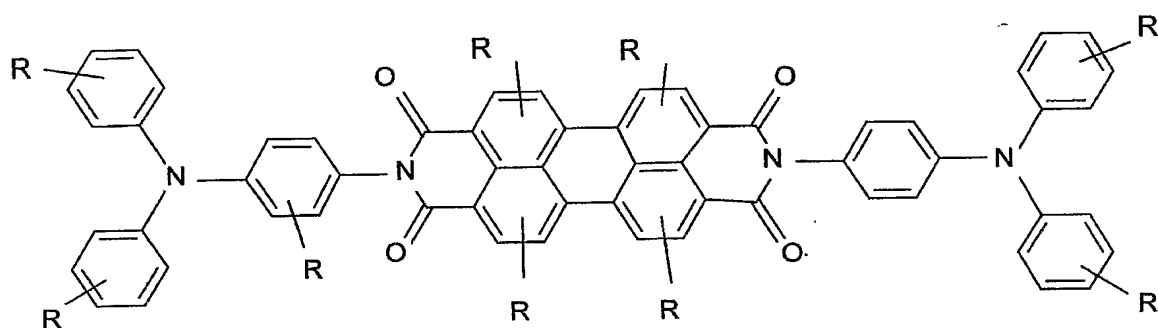


Fig. 4e

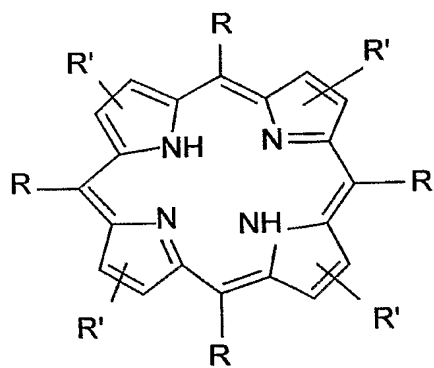


Fig. 4f

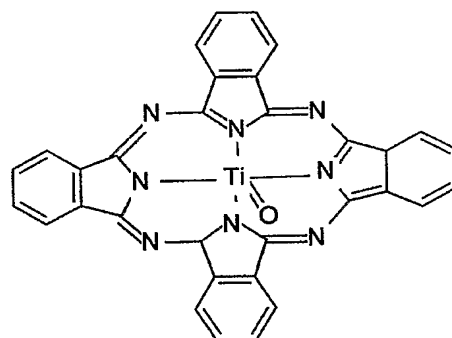


Fig. 4g

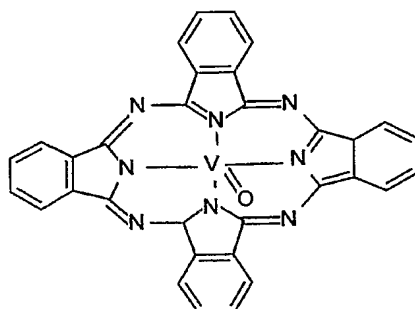


Fig. 4h

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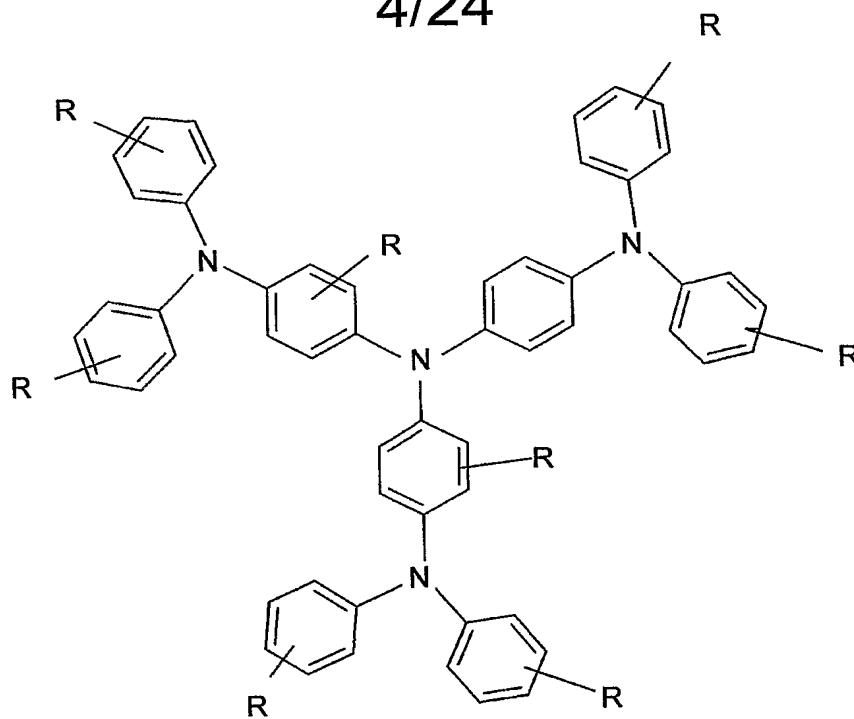


Fig. 4i

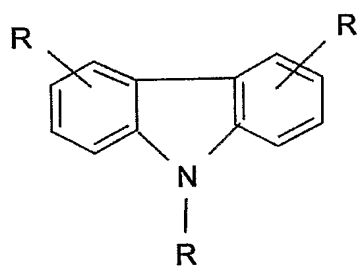


Fig. 4j

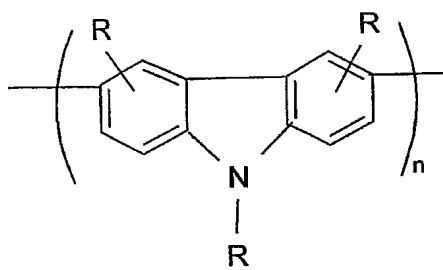


Fig. 4k

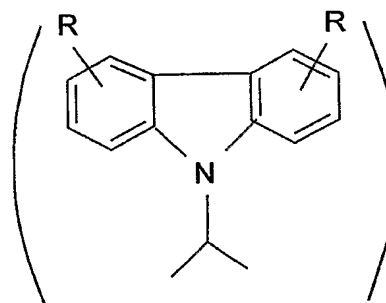


Fig. 4l

5/24

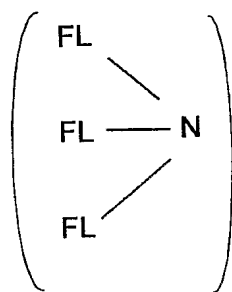


Fig. 5a

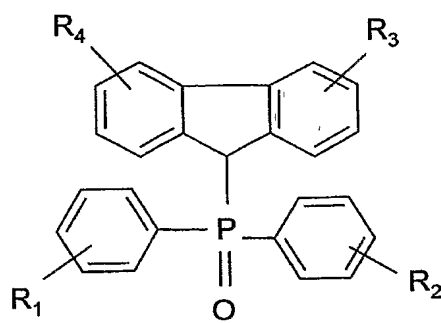


Fig. 5b

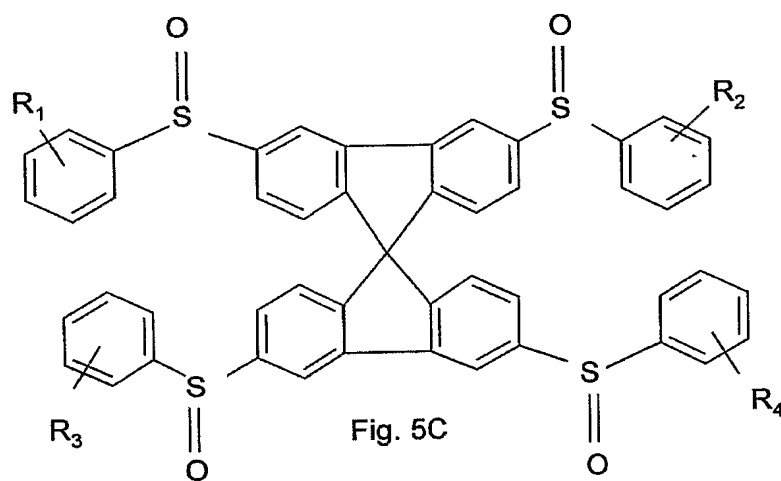


Fig. 5c

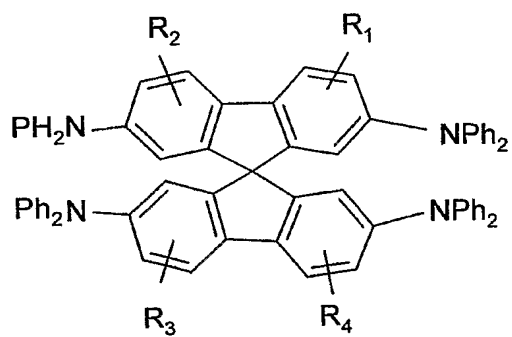


Fig. 5d



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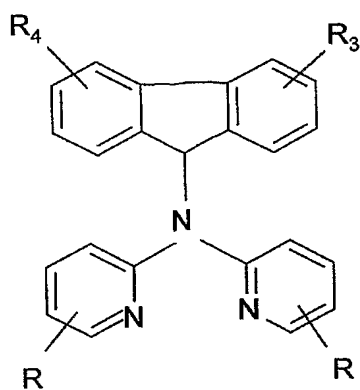


Fig. 5e

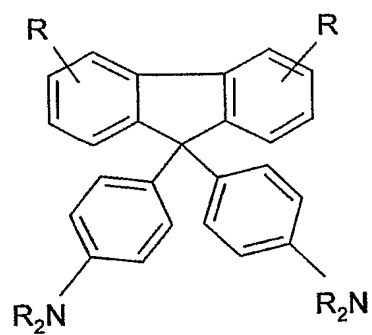


Fig 5f

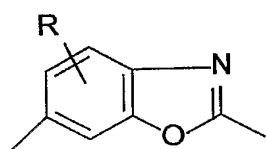


Fig. 6a

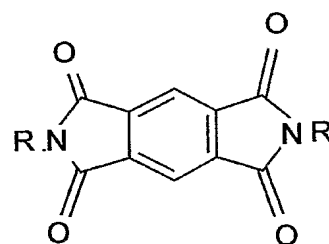


Fig 6b

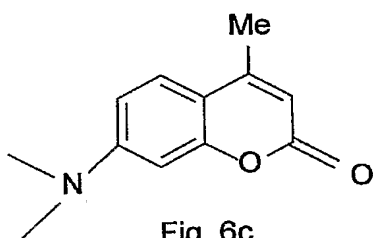


Fig. 6c

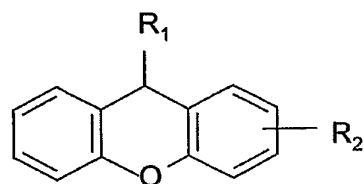


Fig. 6d

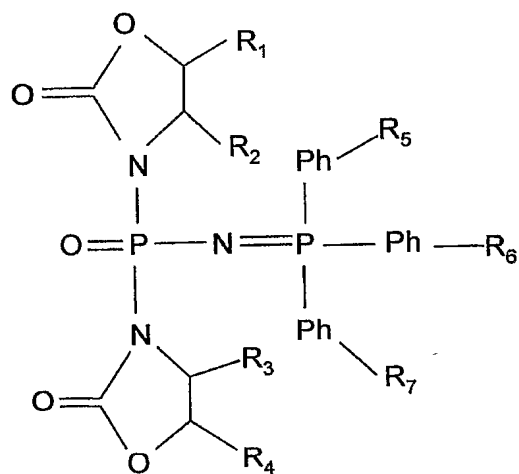


Fig. 6e

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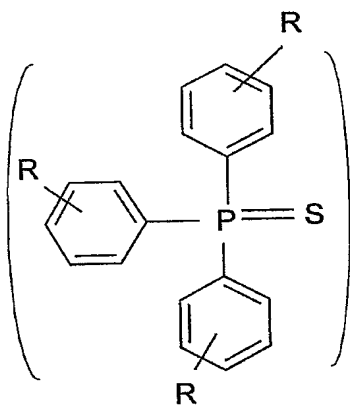


Fig. 7a

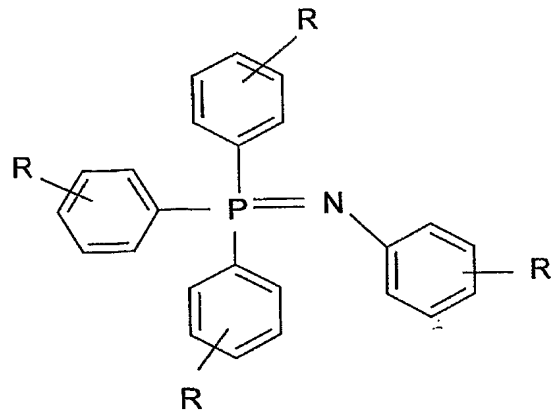


Fig. 7b

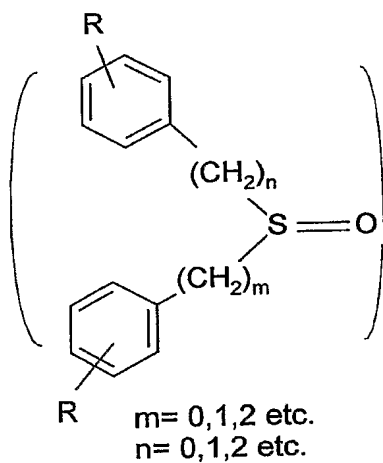


Fig. 7c

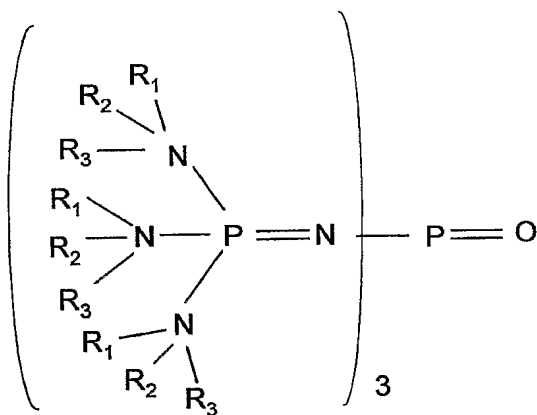


Fig. 7d

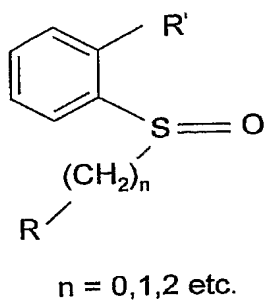


Fig. 7e

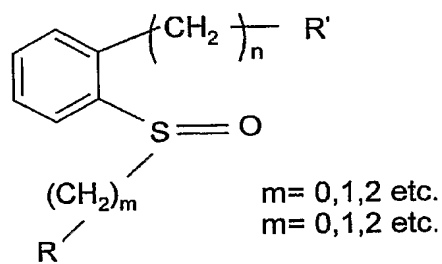


Fig. 7f

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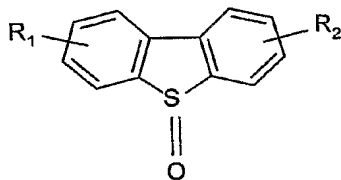


Fig. 8a

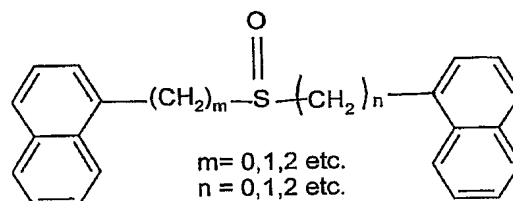


Fig. 8b

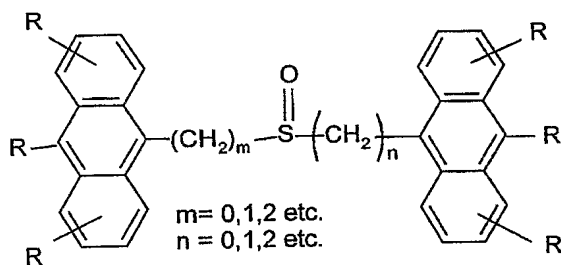


Fig. 8c

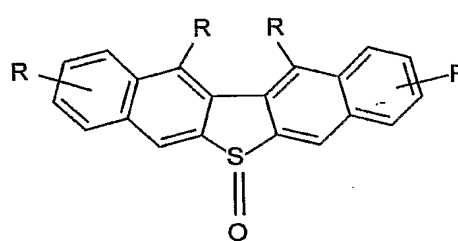


Fig. 8d

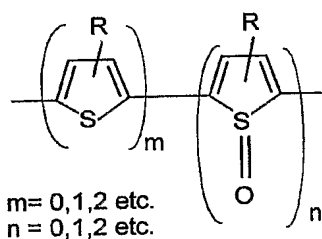


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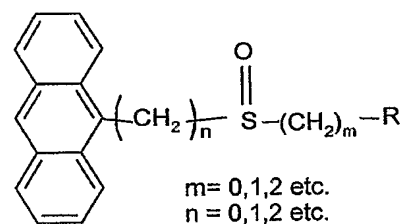


Fig. 8f

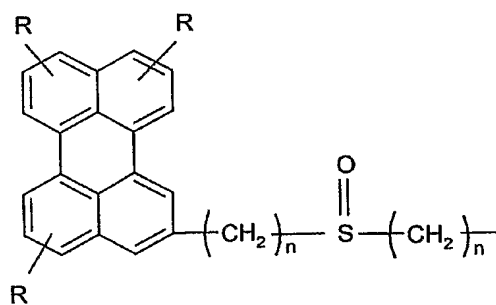


Fig. 8g

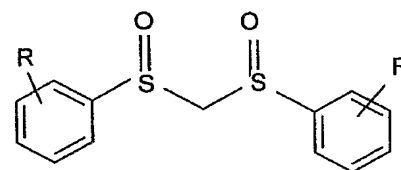
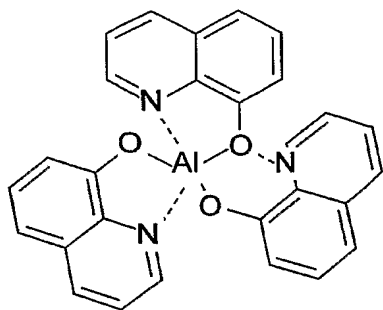
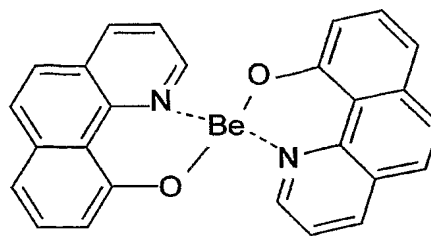


Fig. 8h

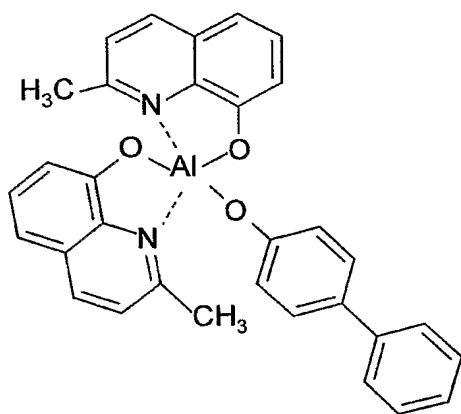
9/24



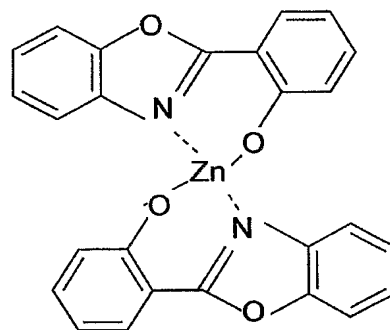
Alq



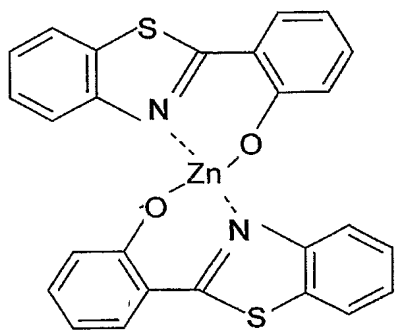
Bebq



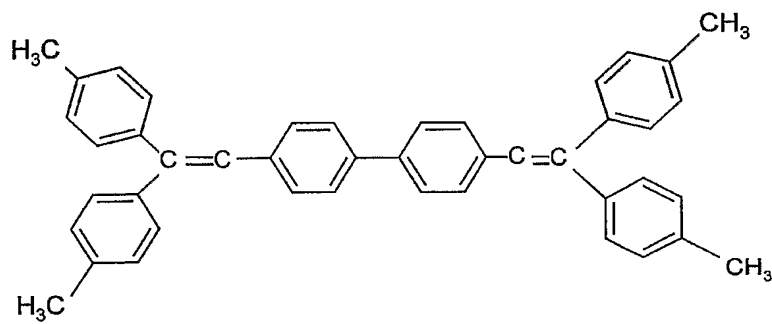
BAlq1



ZnPBO



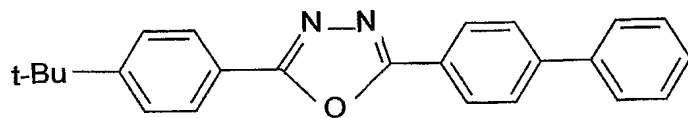
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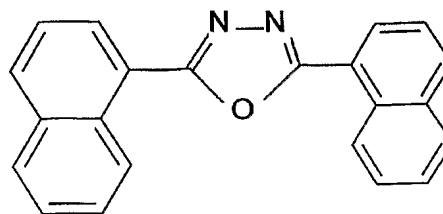
DTVb1

Fig. 9

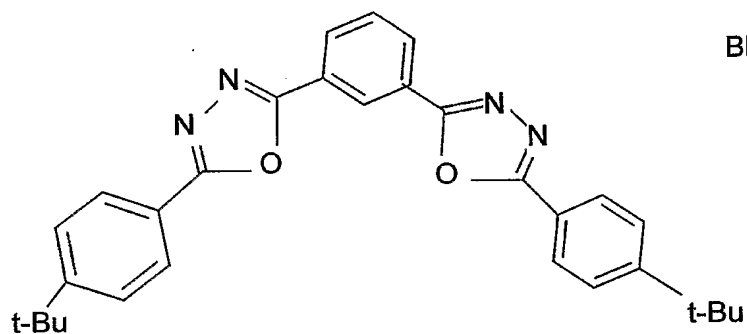
10/24



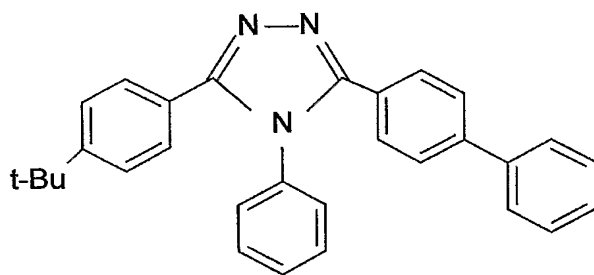
t-Bu-PBD



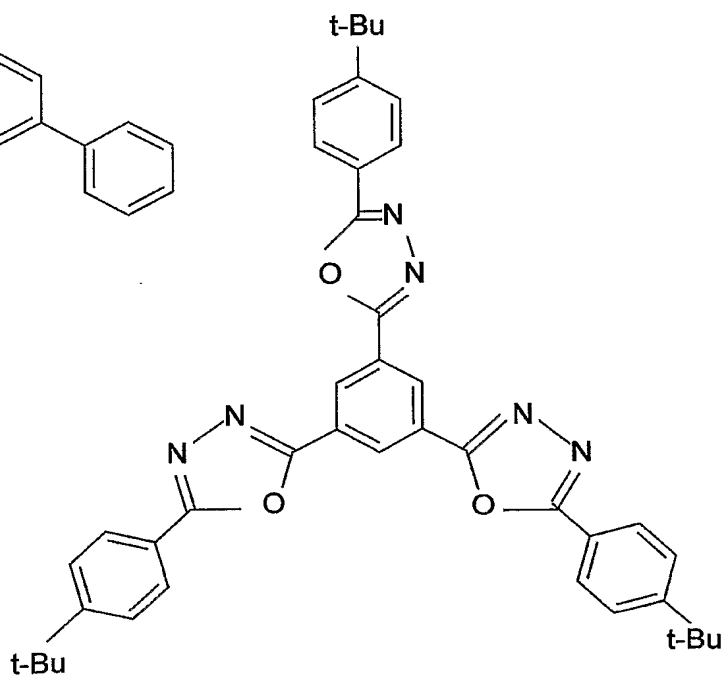
BND



OXD-7



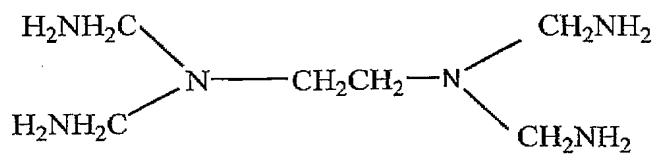
TAZ



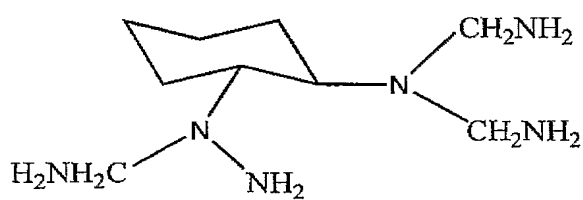
OXD-Star

Fig. 10

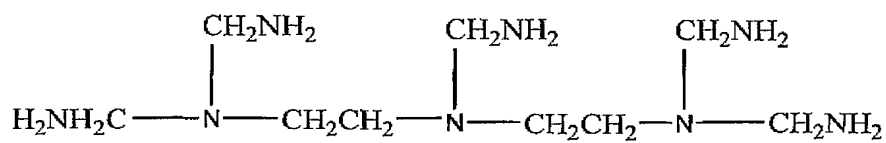
11/24



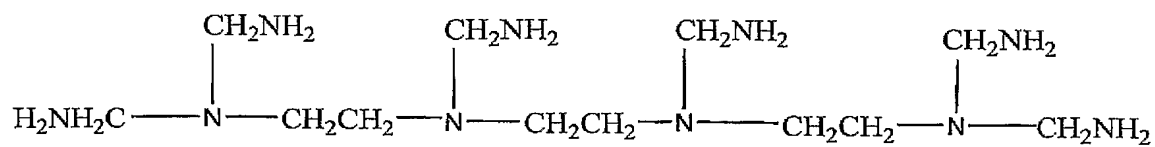
EDTA



DCTA



DTPA



TTHA

Fig. 11

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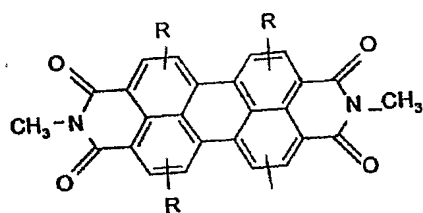


Fig. 12a

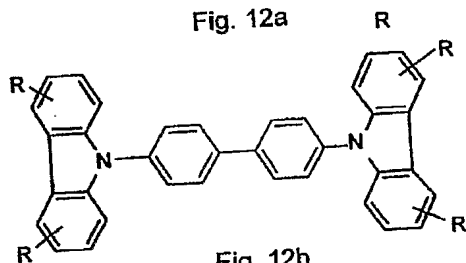


Fig. 12b

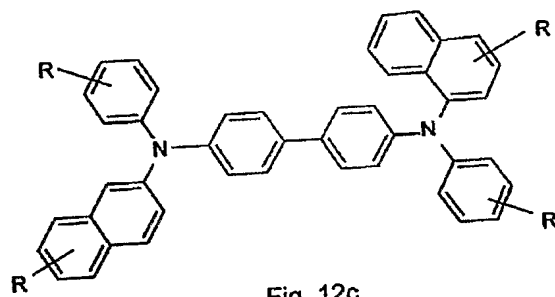


Fig. 12c

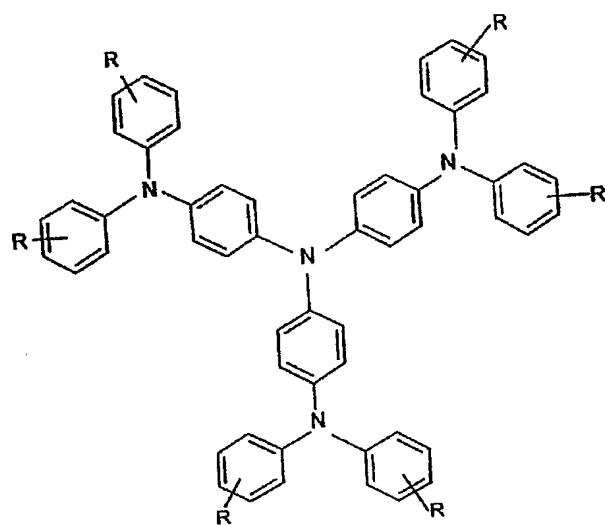


Fig. 12d

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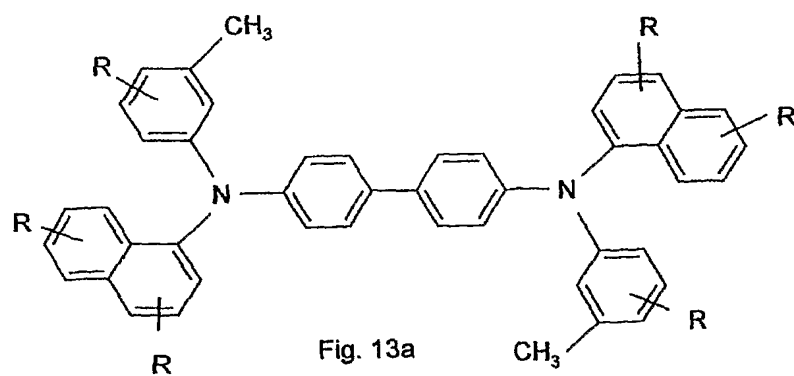


Fig. 13a

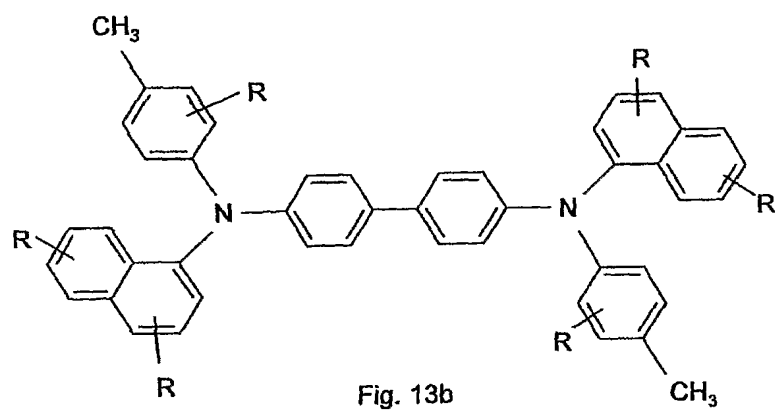


Fig. 13b

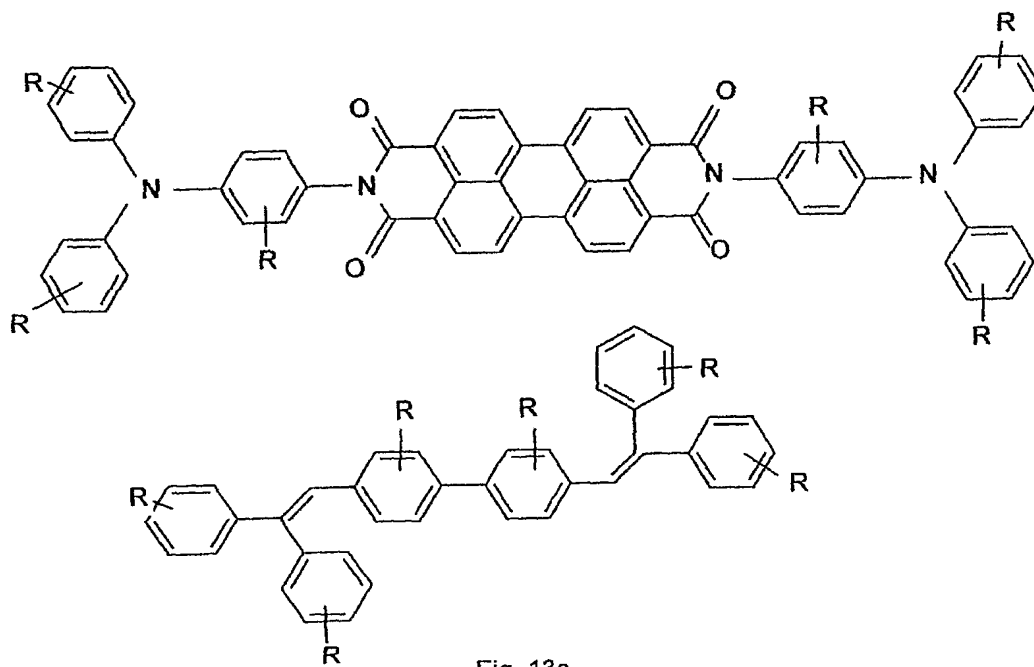


Fig. 13c



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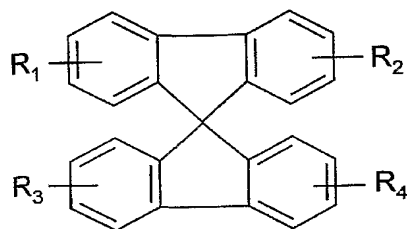


Fig. 14a

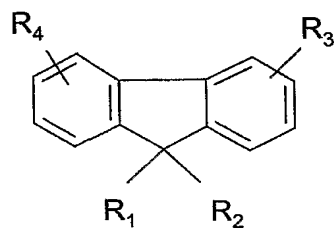
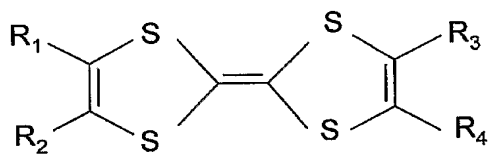


Fig. 14b



or

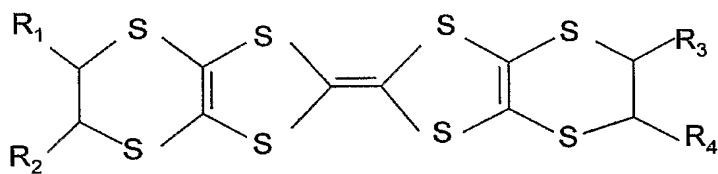


Fig. 14c

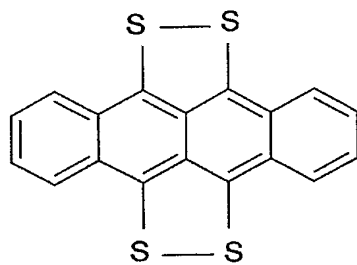


Fig. 14d

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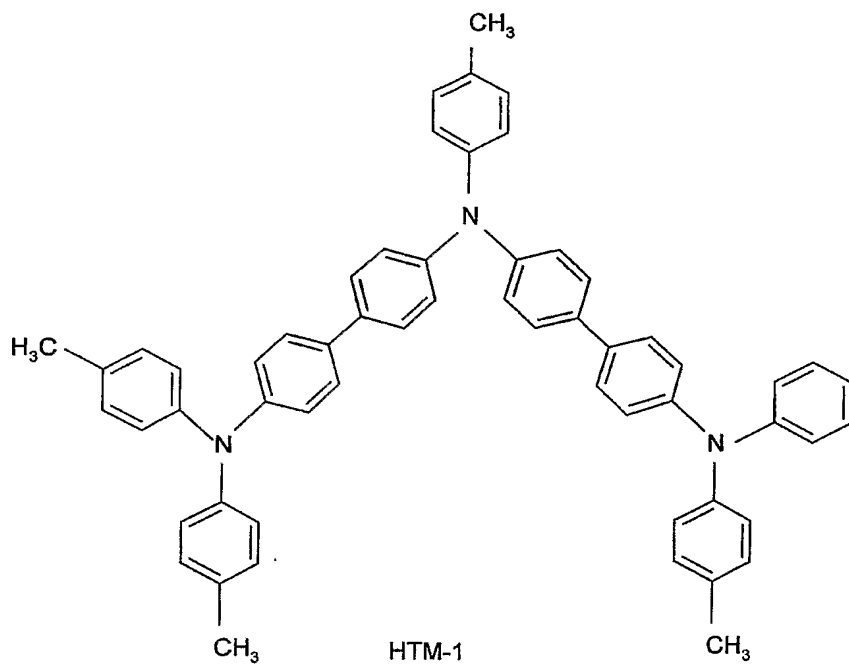


Fig. 15a

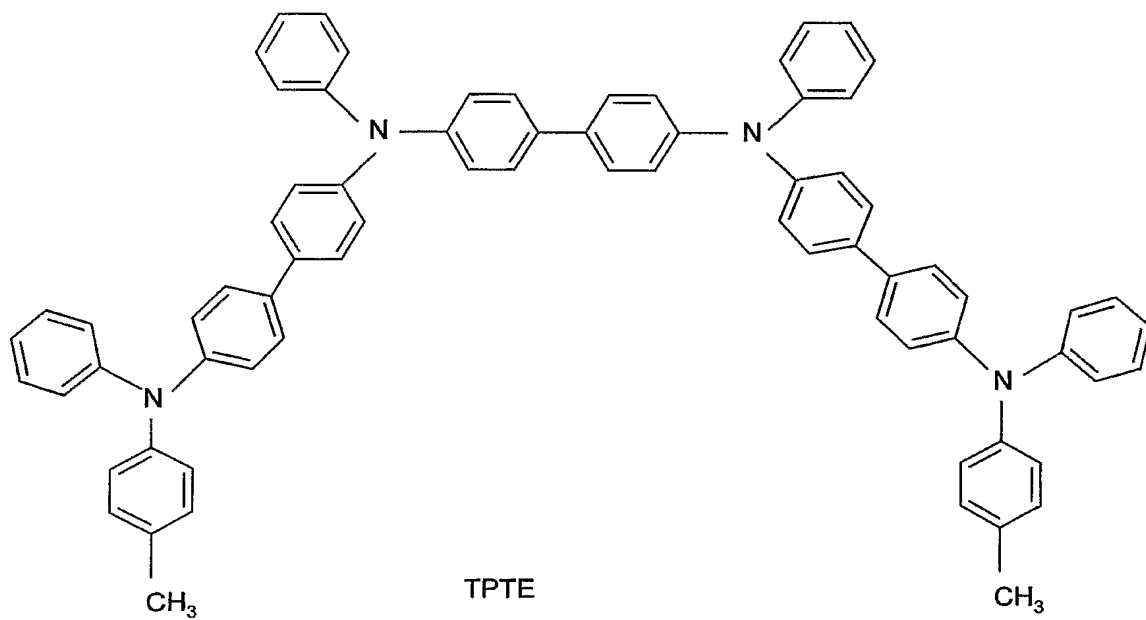


Fig. 15b

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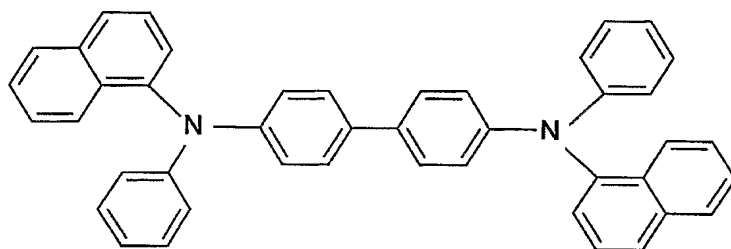
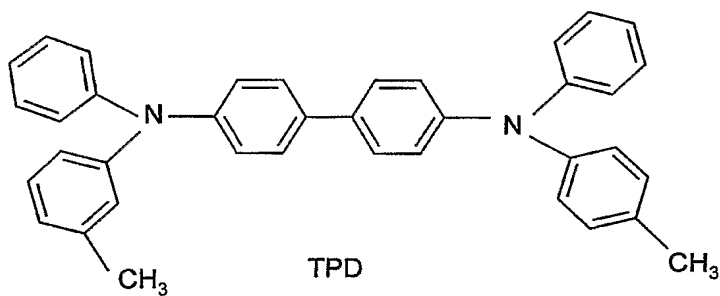
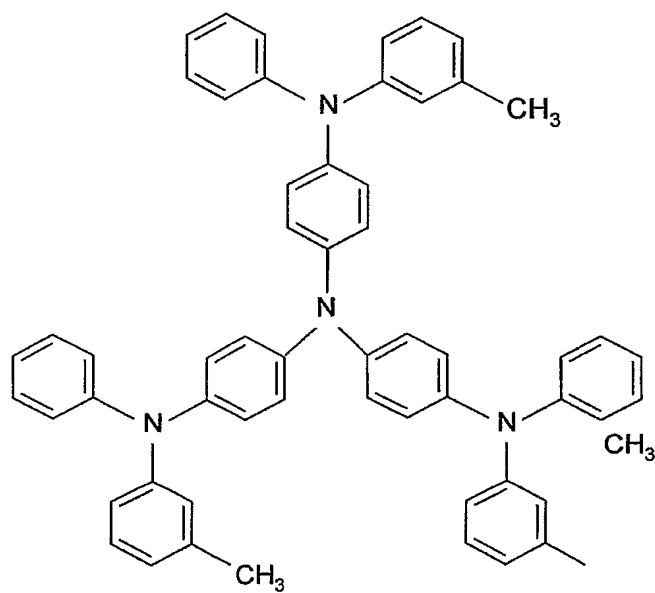
 $\alpha$ -NPB

Fig. 16a



TPD

Fig. 16b



mTADATA

Fig. 16c

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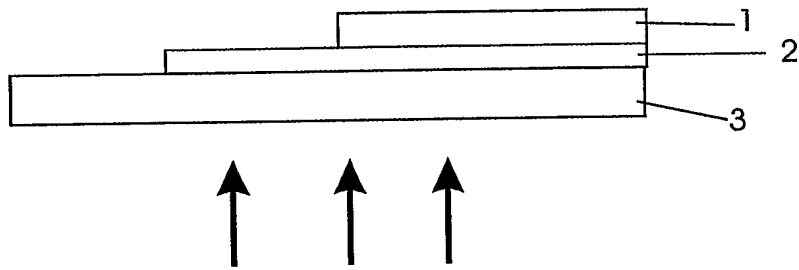


Fig. 17

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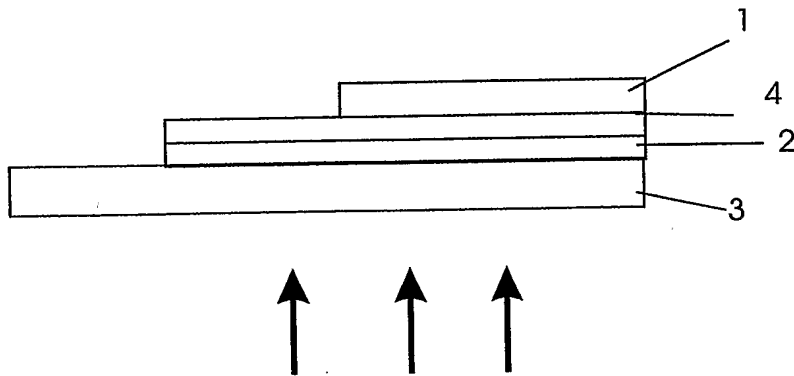


Fig. 18

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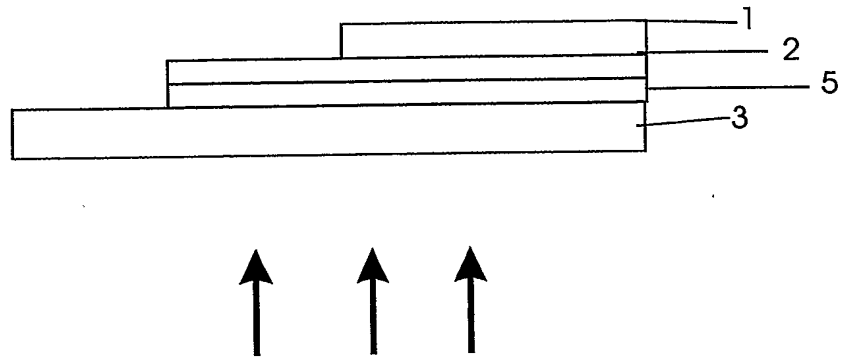


Fig. 19

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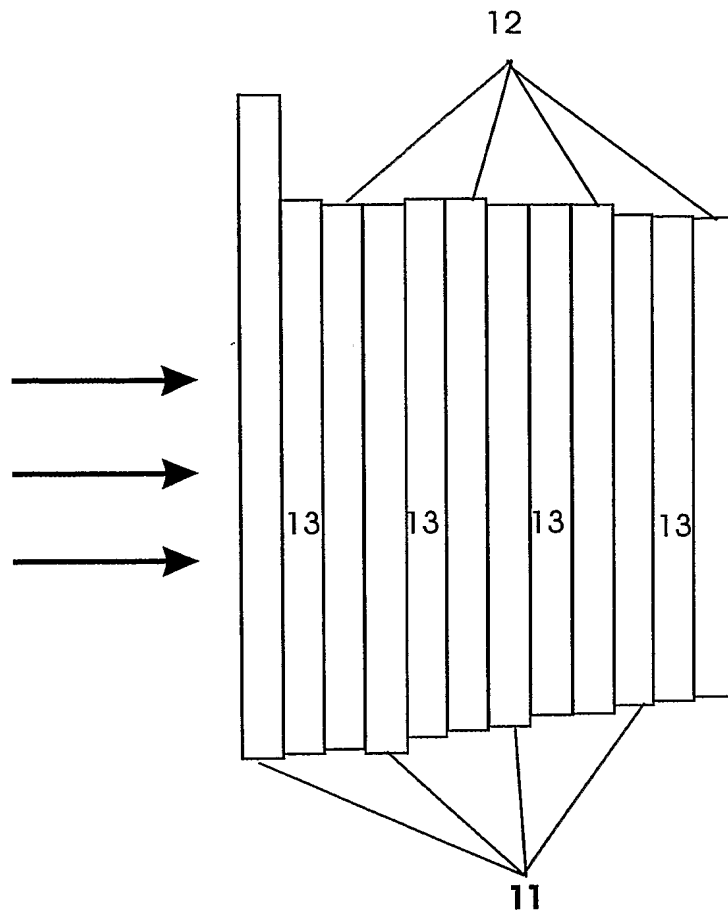


Fig. 20

Photovoltaic IV Measurement on  $\text{Eu}(\text{DBM})_3\text{OPNP}$

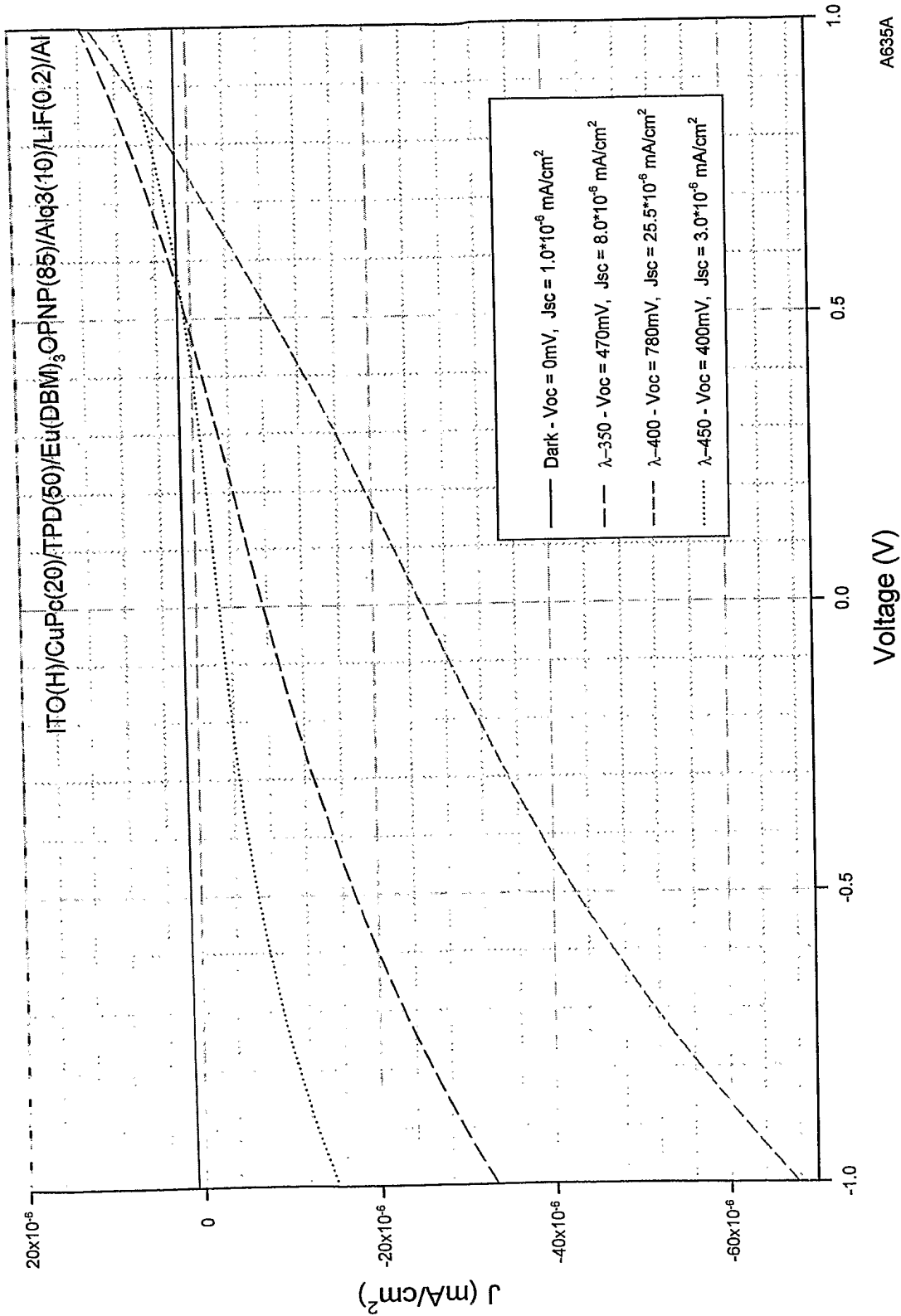


Fig. 21



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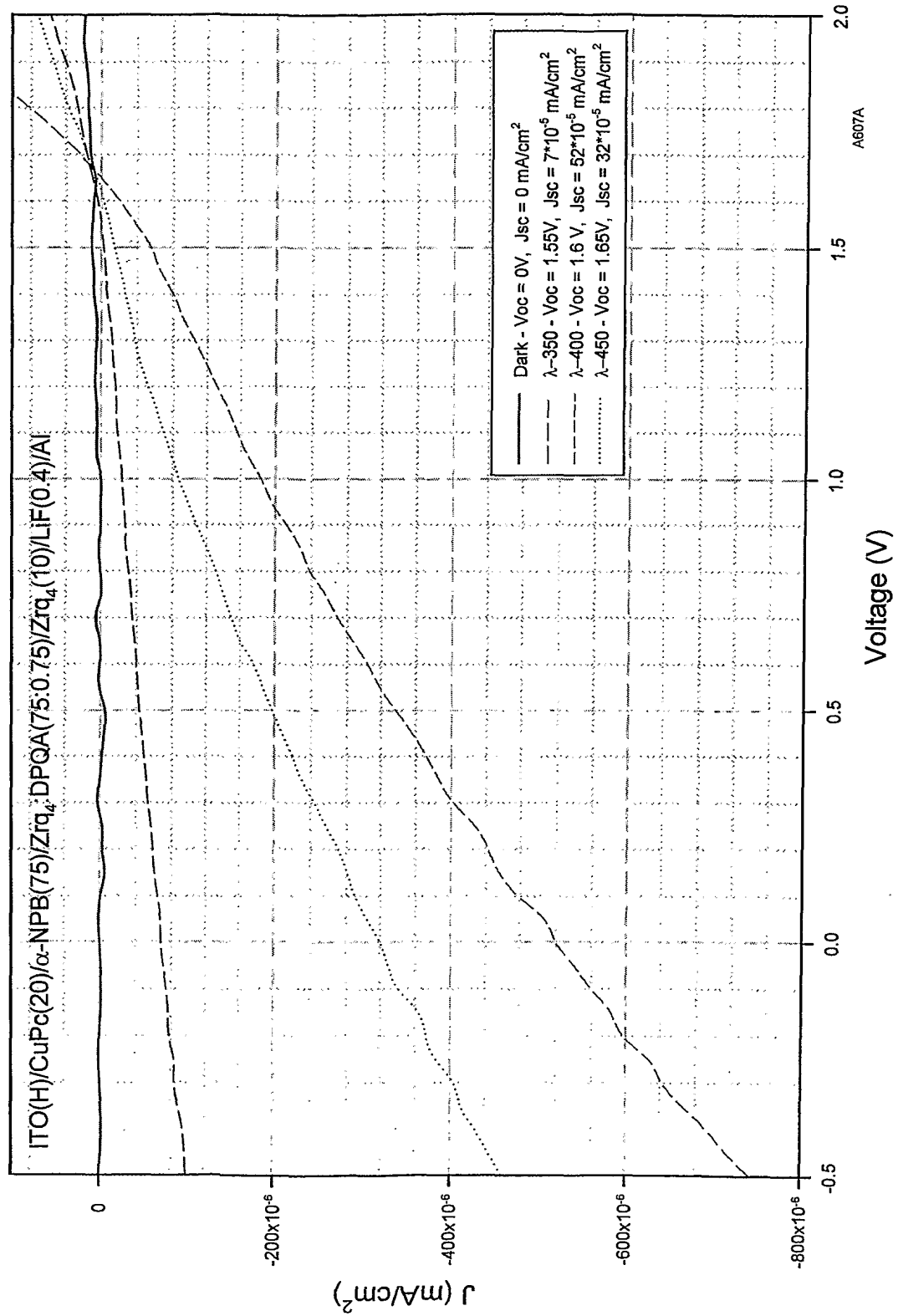
Photovoltaic IV Measurement on  $\text{ZrQ}_4$ 

Fig. 22

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## Photovoltaic IV Measurement on Liq

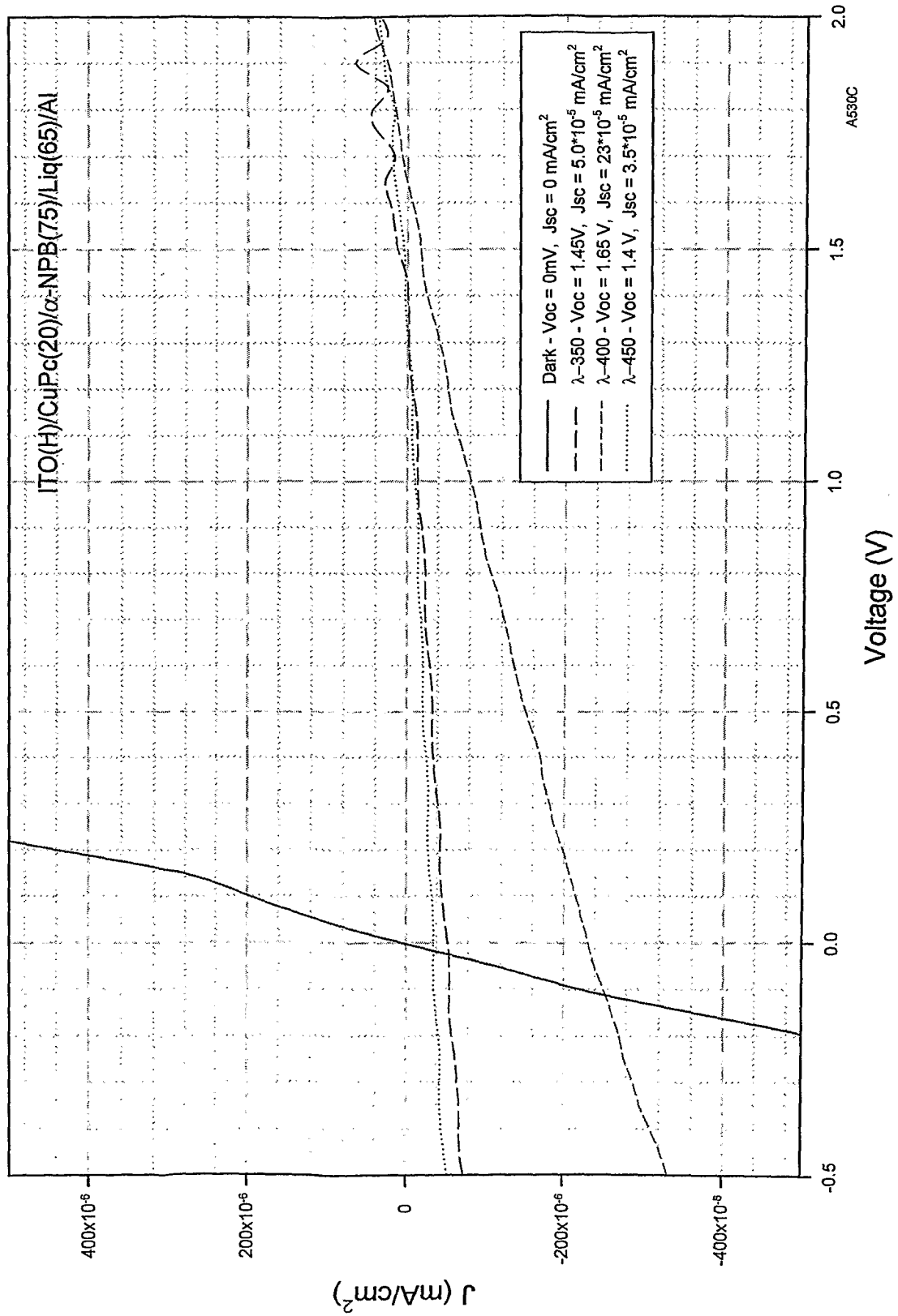


Fig. 23

Photovoltaic IV Measurement on Liq

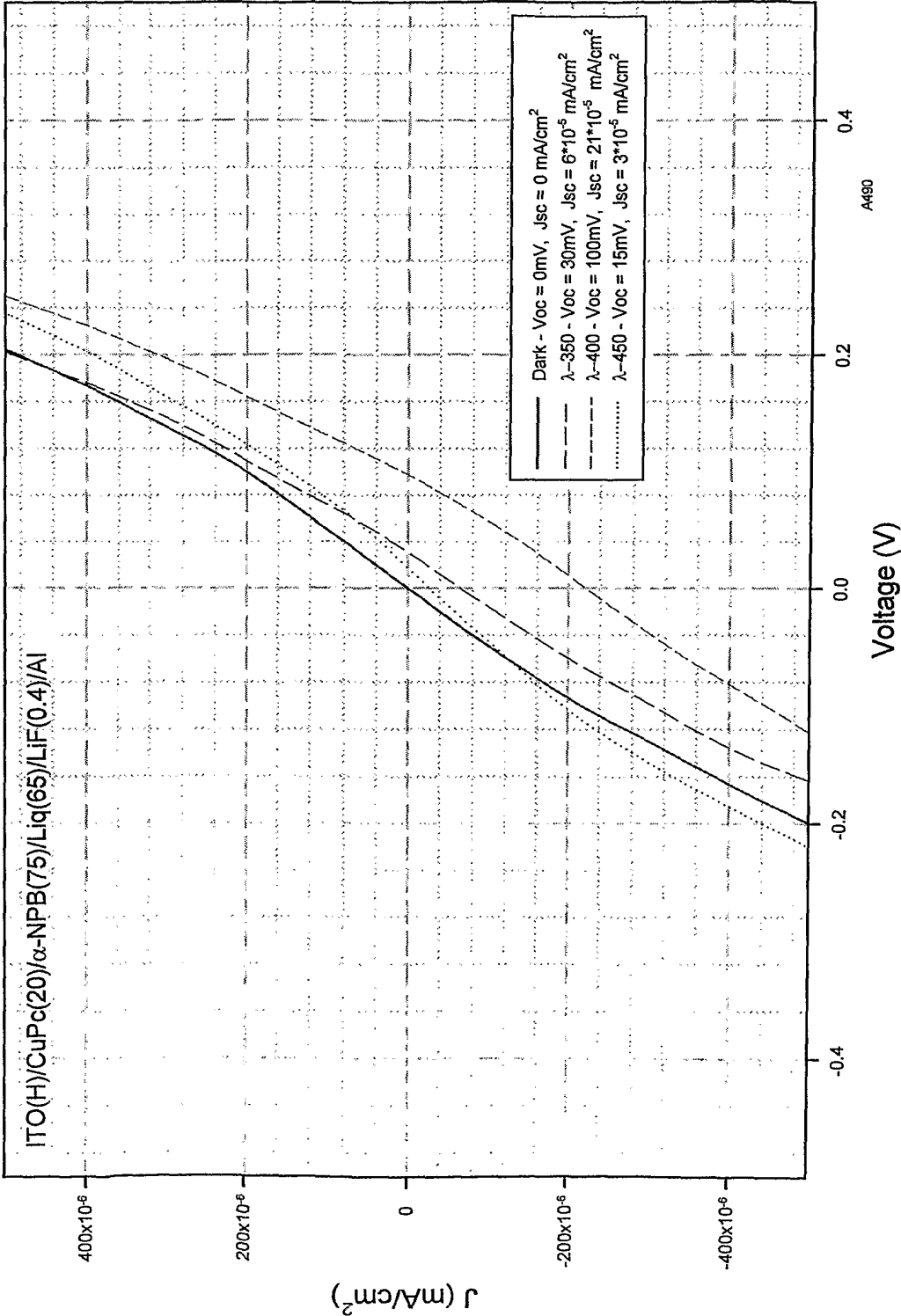


Fig. 24

**DERWENT-ACC-NO:** 2004-143133

**DERWENT-WEEK:** 200629

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**TITLE:** Photovoltaic device such as solar cell, comprises metal chelate as photovoltaic element

**INVENTOR:** ANTIPAN-LARA J; KATHIRGAMANATHAN P ;  
PARTHEEPAN A

**PATENT-ASSIGNEE:** ELAM LTD[ELAMN]

**PRIORITY-DATA:** 2002GB-016154 (July 12, 2002)

**PATENT-FAMILY:**

<b>PUB-NO</b>	<b>PUB-DATE</b>	<b>LANGUAGE</b>
WO 2004008554 A2	January 22, 2004	EN
AU 2003281003 A1	February 2, 2004	EN
AU 2003281003 A8	November 3, 2005	EN

**DESIGNATED-STATES:** AE AG AL AM AT AU AZ BA BB BG  
BR BY BZ CA CH CN CO CR CU CZ  
DE DK DM DZ EC EE ES FI GB GD  
GE GH GM HR HU ID IL IN IS JP  
KE KG KP KR KZ LC LK LR LS LT  
LU LV MA MD MG MK MN MW MX MZ  
NO NZ OM PH PL PT RO RU SD SE S  
G SK SL TJ TM TN TR TT TZ UA UG  
US UZ VN YU ZA ZM ZW AT BE BG  
CH CY CZ DE DK EA EE ES FI FR  
GB GH GM GR HU IE IT KE LS LU  
MC MW MZ NL OA PT RO SD SE SI

SK SL SZ TR TZ UG ZM ZW

**APPLICATION-DATA:**

<b>PUB-NO</b>	<b>APPL-DESCRIPTOR</b>	<b>APPL-NO</b>	<b>APPL-DATE</b>
WO2004008554A2	N/A	2003WO- GB03035	July 14, 2003
AU2003281003A1	N/A	2003AU- 281003	July 14, 2003
AU2003281003A8	Based on	2003AU- 281003	July 14, 2003

**INT-CL-CURRENT:**

<b>TYPE</b>	<b>IPC DATE</b>
CIPS	H01L51/00 20060101
CIPS	H01L51/30 20060101

**ABSTRACTED-PUB-NO:** WO 2004008554 A2**BASIC-ABSTRACT:**

NOVELTY - The photovoltaic device comprises metal chelate (3-12) as photovoltaic element.

USE - Photovoltaic cells such as solar cells for converting solar radiation into usable electrical energy.

ADVANTAGE - The metal chelates absorbs light of

specific wavelength(s) depending on metal and ligands used. The photocurrent output of solar cell is maximized by increasing total number of photons of different energy and wavelength. A wide range of visible spectrum can be obtained by providing several layers of different metal chelate which absorb light of different wavelengths. The metal chelates also absorb light in infrared, ultraviolet or shorter wavelengths, thereby improving utilization of sunlight and increasing power achievable by solar cell.

DESCRIPTION OF DRAWING(S) - The graph shows the relationship of voltage and current measured when photovoltaic device is exposed to light of various wavelengths.

#### **EQUIVALENT-ABSTRACTS:**

##### ORGANIC CHEMISTRY

Preferred Device: The photovoltaic device comprises a first electrode comprising a metal, the photovoltaic element and second electrode, provided sequentially. The second electrode is a transparent substrate which is a conductive glass or plastic material and covers at least a portion of photovoltaic element.

Preferred Element: The photovoltaic element comprises organometallic complex of formula (1) or (2) or binuclear, trinuclear, or polynuclear organometallic complexes of formulae (3-12).

(L $\alpha$ )<sub>n</sub>M (1a)

(L $\alpha$ )<sub>n</sub>M-L<sub>p</sub> (1b)

M = rare earth, non-rare earth, transition, lanthanide or actinide metals preferably samarium (III), europium (II), europium (III), terbium (III), dysprosium (III), ytterbium (III), lutetium (III), gadolinium (III), uranium (III), thulium (III), cerium (III), praseodymium (III), neodymium (III), promethium (III), holmium (III) and erbium (III) or lithium, sodium, potassium, rubidium, cesium, beryllium, magnesium, calcium, strontium, barium, copper, silver, gold, zinc, cadmium, boron, aluminum, gallium, indium, germanium, tin, antimony, manganese, iron, ruthenium, osmium, cobalt, nickel, palladium, platinum, cadmium, chromium, titanium, vanadium, zirconium, tantalum, molybdenum, rhodium, iridium, titanium, niobium, scandium or yttrium, lead;

n = valency of M;

L $\alpha$  and L $\rho$  = organic ligands.

(Ln) $_n$ M $_1$ M $_2$  (2a)

(Ln) $_n$ M $_1$ M $_2$ (L $\rho$ ) (2b)

Ln = L $\alpha$ ;

L $\rho$  = neutral ligand;

M $_1$  = rare earth, transition metal, lanthanide or actinide;

M $_2$  = non-rare earth metal;

n = valency of M $_1$  and M $_2$ .

(L $_m$ ) $_x$ M $_1$ -M $_2$ (Ln) $_y$  (3)

L = bridging ligand;

M1 = rare earth metal;

M2 = M1 or non-rare earth metal;

L<sub>m</sub>, L<sub>n</sub> = L<sub>alpha</sub>;

x = valency of M1;

y = valency of M2.

(L<sub>m</sub>)<sub>x</sub>M1-M3(L<sub>n</sub>)<sub>y</sub>-M2(L<sub>p</sub>)<sub>z</sub> (5)

M1, M2, M3 = same or different rare earth metal;

L<sub>p</sub> = L<sub>alpha</sub>;

z = valency of M3.

M1-M2-M3-M4 (9)

M1-M2-M4-M3 (10)

M4 = M1; and

L = bridging ligand, where rare earth and non-rare earth metal are joined by metal to metal bond and/or via an intermediate bridging atom such that ligand or molecular group of more than 3 metals are joined by metal to metal bond and/or via intermediate ligands.

The organic metallic chelate is a metal quinolate preferably lithium quinolate, aluminum quinolate, scandium quinolate, zirconium quinolate, hafnium quinolate or vanadium quinolate, doped with



fluorescent, phosphorescent or ion fluorescent compound. The dopant is preferably diphenylquinacridine, diphenylquinacridone, coumarins, perylene or their derivatives. The photovoltaic element preferably has structure of formula (IA).

$M = M1$ ; and

R1-R3 = H, optionally substituted hydrocarbyl, aliphatic groups, aromatic groups, heterocyclic and polycyclic ring structures, fluorocarbons and trifluoromethyl, halogens and thiophenyl groups.

A photovoltaic device was fabricated on a clean and dried ITO (indium tin oxide) coated glass piece by sequentially forming layers by vacuum evaporation to form a structure, ITO/CuPc(20 nm)/TPD(50 nm)/Eu(DBM)3(OPNP)/85 nm Alq3/LiF(0.4 nm)/Al, where CuPc is copper phthalocyanine, TPD is N,N'-diphenyl-N,N'-bis (3-methylphenyl)-1,1'-biphenyl -4,4' -diamine, Alq3 is aluminum quinolate, LiF is lithium fluoride and Al is aluminum. The organic coating on the portion etched with concentrated hydrochloric acid was wiped with a cotton bud. The coated electrodes were stored in a vacuum desiccator over a molecular sieve and phosphorous pentoxide, until they were loaded into a vacuum coater and contacted with aluminum top. The active area of the photovoltaic device was 0.08 cm by 0.1 cm<sup>2</sup>. The devices were then kept in a vacuum desiccator and photovoltaic studies were performed. The device was connected to an electric circuit and exposed to light of various wavelengths and the voltage and current were measured. The results were shown graphically where the open circuit voltage  $V_{oc}$  and short circuit current  $J_{sc}$  were plotted.

**CHOSEN-DRAWING:** Dwg.21/24

**TITLE-TERMS:** PHOTOVOLTAIC DEVICE SOLAR CELL  
COMPRISE METAL CHELATE ELEMENT

**DERWENT-CLASS:** E11 E12 L03 U11 U12 X15

**CPI-CODES:** E05-A; E05-B; E05-C; E05-D; E05-F;  
E05-G; E05-J; E05-K; E05-L; E05-M;  
E05-N; E05-P; E05-Q; L03-E05B;

**EPI-CODES:** U11-A01X; U12-A02A2X;

**CHEMICAL-CODES:** Chemical Indexing M3 \*01\*  
Fragmentation Code A103 A960 C710  
D021 D621 H4 H401 H441 H8 M280  
M320 M411 M511 M520 M530 M540 M630  
M781 Q454 R043 Specific Compounds  
RA22LX Registry Numbers 300121

Chemical Indexing M3 \*02\*  
Fragmentation Code A313 A960 C710  
D021 D621 H4 H401 H441 H8 M280  
M320 M411 M511 M520 M530 M540 M630  
M781 Q454 R043 Specific Compounds  
R20372 RA2QMS Registry Numbers  
134570 14922 332819

Chemical Indexing M3 \*03\*  
Fragmentation Code A421 A960 C710  
D021 D621 H4 H401 H441 H8 M280  
M320 M411 M511 M520 M530 M540 M630  
M781 Q454 R043 Specific Compounds  
RA1YYH Registry Numbers 295190

Chemical Indexing M3 \*04\*  
Fragmentation Code A540 A960 C710  
D021 D621 H4 H401 H441 H8 M280  
M320 M411 M511 M520 M530 M540 M630  
M781 Q454 R043 Specific Compounds

# RA1YYI Registry Numbers 295191

Chemical Indexing M3 \*05\*

Fragmentation Code A672 A960 C710  
D021 D621 H4 H401 H441 H8 M280  
M320 M411 M511 M520 M530 M540 M630  
M781 Q454 R043 Specific Compounds  
RACAHJ Registry Numbers 806835

Chemical Indexing M3 \*06\*

Fragmentation Code A765 A960 B515  
B701 B720 B730 B731 B744 B815 B832  
C710 G010 G019 G100 J582 M121 M129  
M144 M148 M149 M210 M214 M233 M262  
M280 M282 M311 M320 M321 M342 M382  
M391 M411 M510 M520 M530 M533 M540  
M620 M630 M781 Q454 R043 Specific  
Compounds RA0480 Registry Numbers  
205837

Chemical Indexing M3 \*07\*

Fragmentation Code A765 A960 A970  
B605 B720 B732 B770 B803 B831 C710  
F011 F019 F511 F599 H213 J582 M210  
M211 M262 M280 M282 M311 M320 M321  
M342 M382 M391 M411 M510 M520 M523  
M530 M540 M620 M630 M781 Q454 R043  
Specific Compounds RAD3HF Registry  
Numbers 845952

Chemical Indexing M3 \*08\*

Fragmentation Code A677 A923 A960  
F011 F012 F013 F014 F015 F019 F431  
F499 F512 G010 G011 G019 G100 H211  
J521 J581 L941 M113 M119 M121 M144  
M210 M211 M215 M233 M240 M262 M280  
M281 M320 M411 M510 M521 M522 M531  
M532 M540 M630 M650 M781 Q454 R043

Specific Compounds RAD3HH Registry  
Numbers 845954

## Chemical Indexing M3 \*09\*

Fragmentation Code						
A103	A111	A119				
A137	A155	A204	A212	A220	A238	A256
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A758	A759	A760	A761	A762	A763	A764
A765	A766	A767	A768	A769	A770	A771
A892	A940	A960	A970	B115	B134	B415
B434	B505	B515	B534	B605	B615	B634
B701	B711	B712	B713	B720	B741	B742
B751	B752	B760	B770	B791	B799	B803
B815	B831	C000	C101	C106	C107	C108
C116	C216	C316	C710	C800	C801	C802
C803	C804	C805	C806	C807	D010	D011
D012	D013	D019	D020	D021	D022	D029
D040	D049	D621	D622	E600	F011	F012
F013	F014	F015	F019	F020	F021	F029
F211	F512	G001	G002	G010	G011	G012
G013	G014	G015	G016	G019	G020	G021
G022	G029	G030	G040	G050	G100	G111
G112	G113	G221	G299	G553	G563	H100
H101	H141	H142	H211	H401	H402	H441
H442	H521	H541	H542	H543	H581	H582
H583	H601	H607	H608	H609	H621	H641
H642	H643	H681	H682	H683	H685	H689
H715	H721	H722	J011	J012	J013	J111
J112	J131	J132	J133	J151	J171	J172
J173	J211	J241	J242	J271	J272	J411
J471	J472	J490	J521	J581	J582	J598
J599	K130	K199	K352	K399	K442	K499
K810	K830	K850	K899	L145	L352	L353
L355	L399	L410	L420	L431	L499	L512
L531	L532	L560	L599	L650	L941	L999
M111	M112	M113	M114	M115	M116	M119
M121	M122	M123	M124	M125	M126	M129
M131	M135	M136	M139	M141	M143	M144

M147 M148 M149 M150 M210 M211 M212  
M213 M214 M215 M216 M220 M221 M222  
M223 M224 M225 M226 M231 M232 M233  
M280 M311 M312 M313 M314 M315 M316  
M320 M321 M322 M323 M331 M332 M333  
M340 M342 M343 M344 M349 M382 M391  
M392 M393 M411 M510 M511 M512 M513  
M520 M521 M522 M523 M530 M531 M532  
M533 M540 M541 M620 M630 M781 Q454  
R043 Markush Compounds 012117301

## Chemical Indexing M3 \*10\*

Fragmentation Code A313 A331 A332  
A349 A350 A351 A382 A421 A422 A423  
A424 A425 A426 A427 A428 A430 A539  
A540 A541 A542 A544 A545 A546 A548  
A673 A676 A677 A678 A940 A960 A970  
B115 B134 B305 B415 B434 B505 B515  
B534 B605 B615 B634 B701 B711 B712  
B713 B720 B741 B742 B751 B752 B760  
B770 B791 B799 B803 B809 B815 B831  
B832 B834 C000 C101 C106 C107 C108  
C116 C216 C316 C710 C800 C801 C802  
C803 C804 C805 C806 C807 D010 D011  
D012 D013 D019 D020 D021 D022 D029  
D040 D049 D621 D622 E600 F011 F012  
F013 F014 F015 F019 F020 F021 F029  
F211 F512 G001 G002 G010 G011 G012  
G013 G014 G015 G016 G019 G020 G021  
G022 G029 G030 G040 G050 G100 G111  
G112 G113 G221 G299 G553 G563 H100  
H101 H141 H142 H211 H401 H402 H441  
H442 H521 H541 H542 H543 H581 H582  
H583 H601 H607 H608 H609 H621 H641  
H642 H643 H681 H682 H683 H685 H689  
H715 H721 H722 J011 J012 J013 J111  
J112 J131 J132 J133 J151 J171 J172  
J173 J211 J241 J242 J271 J272 J411

J471 J472 J490 J521 J581 J582 J598  
J599 K130 K199 K352 K399 K442 K499  
K810 K830 K850 K899 L145 L352 L353  
L355 L399 L410 L420 L431 L499 L512  
L531 L532 L560 L599 L650 L941 L999  
M111 M112 M113 M114 M115 M116 M119  
M121 M122 M123 M124 M125 M126 M129  
M131 M135 M136 M139 M141 M143 M144  
M147 M148 M149 M150 M210 M211 M212  
M213 M214 M215 M216 M220 M221 M222  
M223 M224 M225 M226 M231 M232 M233  
M280 M311 M312 M313 M314 M315 M316  
M320 M321 M322 M323 M331 M332 M333  
M340 M342 M343 M344 M349 M382 M391  
M392 M393 M411 M510 M511 M512 M513  
M520 M521 M522 M523 M530 M531 M532  
M533 M540 M541 M620 M630 M781 Q454  
R043 Markush Compounds 012117302

## Chemical Indexing M3 \*11\*

Fragmentation Code A103 A111 A119  
A137 A155 A204 A212 A220 A238 A256  
A400 A429 A500 A547 A600 A679 A700  
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A765 A766 A767 A768 A769 A770 A771  
A892 A940 A960 A970 B215 B415 B434  
B505 B515 B534 B605 B615 B634 B701  
B711 B712 B713 B720 B730 B731 B732  
B741 B742 B743 B744 B751 B752 B760  
B770 B791 B799 B803 B815 B832 B833  
B834 C000 C101 C106 C107 C108 C116  
C216 C316 C710 C800 C801 C802 C804  
C805 C806 C807 D010 D011 D012 D013  
D019 D020 D021 D022 D029 D040 D049  
D621 D622 E600 F010 F011 F012 F013  
F014 F015 F019 F020 F021 F029 F211  
F512 F610 F699 G001 G002 G010 G011  
G012 G013 G014 G015 G016 G019 G020

G021	G022	G029	G030	G040	G050	G100
G111	G112	G113	G221	G299	G553	G563
H100	H101	H102	H103	H141	H142	H143
H211	H212	H401	H402	H441	H442	H521
H541	H542	H543	H581	H582	H583	H600
H601	H607	H608	H609	H621	H641	H642
H643	H681	H682	H683	H685	H689	H715
H721	H722	H723	J011	J012	J013	J111
J112	J131	J132	J133	J151	J171	J172
J173	J211	J241	J242	J271	J272	J411
J471	J472	J490	J521	J522	J581	J582
J598	J599	K130	K199	K352	K399	K442
K499	K810	K830	K850	K899	L145	L352
L353	L355	L399	L410	L420	L431	L499
L512	L531	L532	L560	L599	L650	L922
L941	L999	M111	M112	M113	M114	M115
M116	M119	M121	M122	M123	M124	M125
M126	M129	M131	M135	M136	M139	M141
M143	M144	M147	M148	M149	M150	M210
M211	M212	M213	M214	M215	M216	M220
M221	M222	M223	M224	M225	M226	M231
M232	M233	M280	M311	M312	M313	M314
M315	M316	M320	M321	M322	M323	M331
M332	M333	M340	M342	M343	M344	M349
M382	M391	M392	M393	M411	M510	M511
M512	M513	M520	M521	M522	M523	M530
M531	M532	M533	M540	M541	M620	M630
M781	Q454	R043	Markush	Compounds		
012117303						

## Chemical Indexing M3 \*12\*

Fragmentation Code	A313	A331	A332			
A349	A350	A351	A382	A421	A422	A423
A424	A425	A426	A427	A428	A430	A539
A540	A541	A542	A544	A545	A546	A548
A673	A676	A677	A678	A940	A960	A970
B215	B305	B415	B434	B505	B515	B534
B605	B615	B634	B701	B711	B712	B713

B720	B730	B731	B732	B741	B742	B743
B744	B751	B752	B760	B770	B791	B799
B803	B809	B815	B832	B833	B834	C000
C101	C106	C107	C108	C116	C216	C316
C710	C800	C801	C802	C804	C805	C806
C807	D010	D011	D012	D013	D019	D020
D021	D022	D029	D040	D049	D621	D622
E600	F010	F011	F012	F013	F014	F015
F019	F020	F021	F029	F211	F512	F610
F699	G001	G002	G010	G011	G012	G013
G014	G015	G016	G019	G020	G021	G022
G029	G030	G040	G050	G100	G111	G112
G113	G221	G299	G553	G563	H100	H101
H102	H103	H141	H142	H143	H211	H212
H401	H402	H441	H442	H521	H541	H542
H543	H581	H582	H583	H600	H601	H607
H608	H609	H621	H641	H642	H643	H681
H682	H683	H685	H689	H715	H721	H722
H723	J011	J012	J013	J111	J112	J131
J132	J133	J151	J171	J172	J173	J211
J241	J242	J271	J272	J411	J471	J472
J490	J521	J522	J581	J582	J598	J599
K130	K199	K352	K399	K442	K499	K810
K830	K850	K899	L145	L352	L353	L355
L399	L410	L420	L431	L499	L512	L531
L532	L560	L599	L650	L922	L941	L999
M111	M112	M113	M114	M115	M116	M119
M121	M122	M123	M124	M125	M126	M129
M131	M135	M136	M139	M141	M143	M144
M147	M148	M149	M150	M210	M211	M212
M213	M214	M215	M216	M220	M221	M222
M223	M224	M225	M226	M231	M232	M233
M280	M311	M312	M313	M314	M315	M316
M320	M321	M322	M323	M331	M332	M333
M340	M342	M343	M344	M349	M382	M391
M392	M393	M411	M510	M511	M512	M513
M520	M521	M522	M523	M530	M531	M532
M533	M540	M541	M620	M630	M781	Q454



## R043 Markush Compounds 012117304

## Chemical Indexing M3 \*13\*

## Fragmentation Code A103 A111 A119

A137	A155	A204	A212	A220	A238	A256
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A758	A759	A760	A761	A762	A763	A764
A765	A766	A767	A768	A769	A770	A771
A892	A940	A960	A970	B215	B415	B434
B505	B515	B534	B605	B615	B634	B701
B702	B711	B712	B713	B720	B721	B722
B732	B741	B742	B744	B751	B752	B760
B770	B791	B798	B799	B803	B815	B832
B833	B834	C000	C101	C106	C107	C108
C116	C216	C316	C710	C720	C800	C801
C802	C803	C804	C805	C806	C807	D010
D011	D012	D013	D019	D020	D021	D022
D029	D040	D049	D621	D622	E600	F010
F011	F012	F013	F014	F015	F019	F020
F021	F029	F211	F512	G001	G002	G010
G011	G012	G013	G014	G015	G016	G019
G020	G021	G022	G029	G030	G040	G050
G100	G111	G112	G113	G221	G299	G553
G563	H100	H101	H141	H142	H211	H401
H402	H441	H442	H521	H541	H542	H543
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H609	H621	H641	H642	H643	H681	H682
H683	H685	H689	H715	H721	H722	H723
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J133	J151	J171	J172	J173	J211	J241
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L599	L650	L941	L999	M111	M112	M113
M114	M115	M116	M119	M121	M122	M123
M124	M125	M126	M129	M131	M135	M136

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M150 M210 M211 M212 M213 M214 M215  
M216 M220 M221 M222 M223 M224 M225  
M226 M231 M232 M233 M280 M311 M312  
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M323 M331 M332 M333 M340 M342 M343  
M344 M349 M382 M391 M392 M393 M411  
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M523 M530 M531 M532 M533 M540 M541  
M620 M630 M781 Q454 R043 Markush  
Compounds 012117305

Chemical Indexing M3 \*14\*  
Fragmentation Code A313 A331 A332  
A349 A350 A351 A382 A421 A422 A423  
A424 A425 A426 A427 A428 A430 A539  
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A673 A676 A677 A678 A940 A960 A970  
B215 B305 B415 B434 B505 B515 B534  
B605 B615 B634 B701 B702 B711 B712  
B713 B720 B721 B722 B732 B741 B742  
B744 B751 B752 B760 B770 B791 B798  
B799 B803 B809 B815 B832 B833 B834  
C000 C101 C106 C107 C108 C116 C216  
C316 C710 C720 C800 C801 C802 C803  
C804 C805 C806 C807 D010 D011 D012  
D013 D019 D020 D021 D022 D029 D040  
D049 D621 D622 E600 F010 F011 F012  
F013 F014 F015 F019 F020 F021 F029  
F211 F512 G001 G002 G010 G011 G012  
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G022 G029 G030 G040 G050 G100 G111  
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H583 H600 H601 H607 H608 H609 H621  
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H689 H715 H721 H722 H723 J011 J012

J013 J111 J112 J131 J132 J133 J151  
J171 J172 J173 J211 J241 J242 J271  
J272 J411 J471 J472 J490 J521 J581  
J582 J598 J599 K130 K199 K352 K399  
K442 K499 K810 K830 K850 K899 L145  
L352 L353 L355 L399 L410 L420 L431  
L499 L512 L531 L532 L560 L599 L650  
L941 L999 M111 M112 M113 M114 M115  
M116 M119 M121 M122 M123 M124 M125  
M126 M129 M131 M135 M136 M139 M141  
M143 M144 M147 M148 M149 M150 M210  
M211 M212 M213 M214 M215 M216 M220  
M221 M222 M223 M224 M225 M226 M231  
M232 M233 M280 M311 M312 M313 M314  
M315 M316 M320 M321 M322 M323 M331  
M332 M333 M340 M342 M343 M344 M349  
M382 M391 M392 M393 M411 M510 M511  
M512 M513 M520 M521 M522 M523 M530  
M531 M532 M533 M540 M541 M620 M630  
M781 Q454 R043 Markush Compounds  
012117306

## Chemical Indexing M3 \*15\*

Fragmentation Code A103 A111 A119  
A137 A155 A204 A212 A220 A238 A256  
A400 A429 A500 A547 A600 A679 A700  
A758 A759 A760 A761 A762 A763 A764  
A765 A766 A767 A768 A769 A770 A771  
A892 A940 A960 A970 B215 B415 B434  
B505 B515 B534 B605 B615 B634 B701  
B711 B712 B713 B720 B741 B742 B751  
B752 B760 B770 B791 B799 B803 B815  
B831 B832 B833 B834 C000 C101 C106  
C107 C108 C116 C216 C316 C710 C720  
C800 C801 C802 C803 C804 C805 C806  
C807 D000 D010 D011 D012 D013 D019  
D020 D021 D022 D029 D040 D049 D621  
D622 E160 E220 E600 F010 F011 F012

F013	F014	F015	F019	F020	F021	F029
F211	F512	G000	G001	G002	G010	G011
G012	G013	G014	G015	G016	G019	G020
G021	G022	G029	G030	G040	G050	G100
G111	G112	G113	G221	G299	G341	G553
G563	H100	H101	H141	H142	H211	H401
H402	H441	H442	H521	H541	H542	H543
H581	H582	H583	H600	H601	H607	H608
H609	H621	H622	H641	H642	H643	H681
H682	H683	H685	H689	H715	H721	H722
H723	J011	J012	J013	J111	J112	J131
J132	J133	J151	J171	J172	J173	J211
J241	J242	J271	J272	J411	J471	J472
J490	J521	J581	J582	J598	J599	K130
K199	K352	K399	K442	K499	K810	K830
K850	K899	L145	L352	L353	L355	L399
L410	L420	L431	L499	L512	L531	L532
L560	L599	L650	L941	L999	M111	M112
M113	M114	M115	M116	M119	M121	M122
M123	M124	M125	M126	M129	M131	M135
M136	M139	M141	M143	M144	M147	M148
M149	M150	M210	M211	M212	M213	M214
M215	M216	M220	M221	M222	M223	M224
M225	M226	M231	M232	M233	M280	M311
M312	M313	M314	M315	M316	M320	M321
M322	M323	M331	M332	M333	M340	M342
M343	M344	M349	M382	M391	M392	M393
M411	M510	M511	M512	M513	M520	M521
M522	M523	M530	M531	M532	M533	M540
M541	M620	M630	M781	Q454	R043	Ring
Index	Numbers	03480	03524	Markush		
Compounds	01211	7307				

Chemical Indexing M3 \*16\*

Fragmentation	Code	A313	A331	A332		
A349	A350	A351	A382	A421	A422	A423
A424	A425	A426	A427	A428	A430	A539
A540	A541	A542	A544	A545	A546	A548

A673	A676	A677	A678	A940	A960	A970
B215	B305	B415	B434	B505	B515	B534
B605	B615	B634	B701	B711	B712	B713
B720	B741	B742	B751	B752	B760	B770
B791	B799	B803	B809	B815	B831	B832
B833	B834	C000	C101	C106	C107	C108
C116	C216	C316	C710	C720	C800	C801
C802	C803	C804	C805	C806	C807	D000
D010	D011	D012	D013	D019	D020	D021
D022	D029	D040	D049	D621	D622	E160
E220	E600	F010	F011	F012	F013	F014
F015	F019	F020	F021	F029	F211	F512
G000	G001	G002	G010	G011	G012	G013
G014	G015	G016	G019	G020	G021	G022
G029	G030	G040	G050	G100	G111	G112
G113	G221	G299	G341	G553	G563	H100
H101	H141	H142	H211	H401	H402	H441
H442	H521	H541	H542	H543	H581	H582
H583	H600	H601	H607	H608	H609	H621
H622	H641	H642	H643	H681	H682	H683
H685	H689	H715	H721	H722	H723	J011
J012	J013	J111	J112	J131	J132	J133
J151	J171	J172	J173	J211	J241	J242
J271	J272	J411	J471	J472	J490	J521
J581	J582	J598	J599	K130	K199	K352
K399	K442	K499	K810	K830	K850	K899
L145	L352	L353	L355	L399	L410	L420
L431	L499	L512	L531	L532	L560	L599
L650	L941	L999	M111	M112	M113	M114
M115	M116	M119	M121	M122	M123	M124
M125	M126	M129	M131	M135	M136	M139
M141	M143	M144	M147	M148	M149	M150
M210	M211	M212	M213	M214	M215	M216
M220	M221	M222	M223	M224	M225	M226
M231	M232	M233	M280	M311	M312	M313
M314	M315	M316	M320	M321	M322	M323
M331	M332	M333	M340	M342	M343	M344
M349	M382	M391	M392	M393	M411	M510

M511 M512 M513 M520 M521 M522 M523  
M530 M531 M532 M533 M540 M541 M620  
M630 M781 Q454 R043 Ring Index  
Numbers 03480 03524 Markush  
Compounds 012117308

## Chemical Indexing M3 \*17\*

Fragmentation Code A103 A111 A119  
A137 A155 A204 A212 A220 A238 A256  
A400 A429 A500 A547 A600 A679 A700  
A758 A759 A760 A761 A762 A763 A764  
A765 A766 A767 A768 A769 A770 A771  
A892 A940 A960 A970 B215 B415 B434  
B505 B515 B534 B605 B615 B634 B701  
B711 B712 B713 B720 B741 B742 B751  
B752 B760 B770 B791 B799 B803 B815  
B831 C000 C101 C106 C107 C108 C116  
C216 C316 C710 C720 C800 C801 C802  
C803 C804 C805 C806 C807 D010 D011  
D012 D013 D019 D020 D021 D022 D029  
D040 D049 D621 D622 E600 F010 F011  
F012 F013 F014 F015 F016 F019 F020  
F021 F029 F211 F431 F499 F512 G001  
G002 G010 G011 G012 G013 G014 G015  
G016 G019 G020 G021 G022 G029 G030  
G040 G050 G100 G111 G112 G113 G221  
G299 G553 G563 H100 H101 H141 H142  
H211 H401 H402 H441 H442 H521 H541  
H542 H543 H581 H582 H583 H600 H601  
H607 H608 H609 H621 H622 H623 H641  
H642 H643 H681 H682 H683 H685 H689  
H715 H721 H722 H723 J011 J012 J013  
J111 J112 J131 J132 J133 J151 J171  
J172 J173 J211 J241 J242 J271 J272  
J411 J471 J472 J490 J521 J581 J582  
J598 J599 K130 K199 K352 K399 K442  
K499 K810 K830 K850 K899 L145 L352  
L353 L355 L399 L410 L420 L431 L499

L512 L531 L532 L560 L599 L650 L941  
L999 M111 M112 M113 M114 M115 M116  
M119 M121 M122 M123 M124 M125 M126  
M129 M131 M135 M136 M139 M141 M143  
M144 M147 M148 M149 M150 M210 M211  
M212 M213 M214 M215 M216 M220 M221  
M222 M223 M224 M225 M226 M231 M232  
M233 M280 M311 M312 M313 M314 M315  
M316 M320 M321 M322 M323 M331 M332  
M333 M340 M342 M343 M344 M349 M382  
M391 M392 M393 M411 M510 M511 M512  
M513 M520 M521 M522 M523 M530 M531  
M532 M533 M540 M541 M620 M630 M781  
Q454 R043 Markush Compounds  
012117309

## Chemical Indexing M3 \*18\*

Fragmentation Code A313 A331 A332  
A349 A350 A351 A382 A421 A422 A423  
A424 A425 A426 A427 A428 A430 A539  
A540 A541 A542 A544 A545 A546 A548  
A673 A676 A677 A678 A940 A960 A970  
B215 B305 B415 B434 B505 B515 B534  
B605 B615 B634 B701 B711 B712 B713  
B720 B741 B742 B751 B752 B760 B770  
B791 B799 B803 B809 B815 B831 B832  
B834 C000 C101 C106 C107 C108 C116  
C216 C316 C710 C720 C800 C801 C802  
C803 C804 C805 C806 C807 D010 D011  
D012 D013 D019 D020 D021 D022 D029  
D040 D049 D621 D622 E600 F010 F011  
F012 F013 F014 F015 F016 F019 F020  
F021 F029 F211 F431 F499 F512 G001  
G002 G010 G011 G012 G013 G014 G015  
G016 G019 G020 G021 G022 G029 G030  
G040 G050 G100 G111 G112 G113 G221  
G299 G553 G563 H100 H101 H141 H142  
H211 H401 H402 H441 H442 H521 H541

H542 H543 H581 H582 H583 H600 H601  
H607 H608 H609 H621 H622 H623 H641  
H642 H643 H681 H682 H683 H685 H689  
H715 H721 H722 H723 J011 J012 J013  
J111 J112 J131 J132 J133 J151 J171  
J172 J173 J211 J241 J242 J271 J272  
J411 J471 J472 J490 J521 J581 J582  
J598 J599 K130 K199 K352 K399 K442  
K499 K810 K830 K850 K899 L145 L352  
L353 L355 L399 L410 L420 L431 L499  
L512 L531 L532 L560 L599 L650 L941  
L999 M111 M112 M113 M114 M115 M116  
M119 M121 M122 M123 M124 M125 M126  
M129 M131 M135 M136 M139 M141 M143  
M144 M147 M148 M149 M150 M210 M211  
M212 M213 M214 M215 M216 M220 M221  
M222 M223 M224 M225 M226 M231 M232  
M233 M280 M311 M312 M313 M314 M315  
M316 M320 M321 M322 M323 M331 M332  
M333 M340 M342 M343 M344 M349 M382  
M391 M392 M393 M411 M510 M511 M512  
M513 M520 M521 M522 M523 M530 M531  
M532 M533 M540 M541 M620 M630 M781  
Q454 R043 Markush Compounds  
012117310

## Chemical Indexing M3 \*19\*

Fragmentation Code A103 A111 A119  
A137 A155 A204 A212 A220 A238 A256  
A400 A429 A500 A547 A600 A679 A700  
A758 A759 A760 A761 A762 A763 A764  
A765 A766 A767 A768 A769 A770 A771  
A892 A940 A960 A970 B215 B415 B434  
B505 B515 B534 B605 B615 B634 B701  
B711 B712 B713 B720 B741 B742 B751  
B752 B760 B770 B791 B799 B803 B815  
B831 C000 C101 C106 C107 C108 C116  
C216 C316 C710 C800 C801 C802 C804



C805 C806 C807 D010 D011 D012 D013  
D014 D019 D020 D021 D022 D029 D040  
D049 D621 D622 E350 E600 F010 F011  
F012 F013 F014 F015 F019 F020 F021  
F029 F211 F512 G001 G002 G010 G011  
G012 G013 G014 G015 G016 G019 G020  
G021 G022 G029 G030 G040 G050 G100  
G111 G112 G113 G221 G299 G553 G563  
H100 H101 H103 H141 H142 H211 H212  
H401 H402 H441 H442 H521 H541 H542  
H543 H581 H582 H583 H600 H601 H607  
H608 H609 H621 H641 H642 H643 H681  
H682 H683 H685 H689 H715 H721 H722  
H723 J011 J012 J013 J111 J112 J131  
J132 J133 J151 J171 J172 J173 J211  
J241 J242 J271 J272 J411 J471 J472  
J490 J521 J523 J581 J582 J598 J599  
K130 K199 K352 K399 K442 K499 K810  
K830 K850 K899 L145 L352 L353 L355  
L399 L410 L420 L431 L499 L512 L531  
L532 L560 L599 L650 L930 L941 L999  
M111 M112 M113 M114 M115 M116 M119  
M121 M122 M123 M124 M125 M126 M129  
M131 M135 M136 M139 M141 M143 M144  
M147 M148 M149 M150 M210 M211 M212  
M213 M214 M215 M216 M220 M221 M222  
M223 M224 M225 M226 M231 M232 M233  
M280 M311 M312 M313 M314 M315 M316  
M320 M321 M322 M323 M331 M332 M333  
M340 M342 M343 M344 M349 M382 M391  
M392 M393 M411 M510 M511 M512 M513  
M520 M521 M522 M523 M530 M531 M532  
M533 M540 M541 M620 M630 M781 Q454  
R043 Ring Index Numbers 07309  
Markush Compounds 012117311

Chemical Indexing M3 \*20\*  
Fragmentation Code A313 A331 A332

A349	A350	A351	A382	A421	A422	A423
A424	A425	A426	A427	A428	A430	A539
A540	A541	A542	A544	A545	A546	A548
A673	A676	A677	A678	A940	A960	A970
B215	B305	B415	B434	B505	B515	B534
B605	B615	B634	B701	B711	B712	B713
B720	B741	B742	B751	B752	B760	B770
B791	B799	B803	B809	B815	B831	B832
B834	C000	C101	C106	C107	C108	C116
C216	C316	C710	C800	C801	C802	C804
C805	C806	C807	D010	D011	D012	D013
D014	D019	D020	D021	D022	D029	D040
D049	D621	D622	E350	E600	F010	F011
F012	F013	F014	F015	F019	F020	F021
F029	F211	F512	G001	G002	G010	G011
G012	G013	G014	G015	G016	G019	G020
G021	G022	G029	G030	G040	G050	G100
G111	G112	G113	G221	G299	G553	G563
H100	H101	H103	H141	H142	H211	H212
H401	H402	H441	H442	H521	H541	H542
H543	H581	H582	H583	H600	H601	H607
H608	H609	H621	H641	H642	H643	H681
H682	H683	H685	H689	H715	H721	H722
H723	J011	J012	J013	J111	J112	J131
J132	J133	J151	J171	J172	J173	J211
J241	J242	J271	J272	J411	J471	J472
J490	J521	J523	J581	J582	J598	J599
K130	K199	K352	K399	K442	K499	K810
K830	K850	K899	L145	L352	L353	L355
L399	L410	L420	L431	L499	L512	L531
L532	L560	L599	L650	L930	L941	L999
M111	M112	M113	M114	M115	M116	M119
M121	M122	M123	M124	M125	M126	M129
M131	M135	M136	M139	M141	M143	M144
M147	M148	M149	M150	M210	M211	M212
M213	M214	M215	M216	M220	M221	M222
M223	M224	M225	M226	M231	M232	M233
M280	M311	M312	M313	M314	M315	M316

M320 M321 M322 M323 M331 M332 M333  
M340 M342 M343 M344 M349 M382 M391  
M392 M393 M411 M510 M511 M512 M513  
M520 M521 M522 M523 M530 M531 M532  
M533 M540 M541 M620 M630 M781 Q454  
R043 Ring Index Numbers 07309  
Markush Compounds 012117312

Chemical Indexing M3 \*21\*  
Fragmentation Code A103 A111 A119  
A137 A155 A204 A212 A220 A238 A256  
A400 A429 A500 A547 A600 A679 A700  
A758 A759 A760 A761 A762 A763 A764  
A765 A766 A767 A768 A769 A770 A771  
A892 A940 A960 A970 B215 B415 B434  
B505 B515 B534 B605 B615 B634 B701  
B711 B712 B713 B720 B741 B742 B751  
B752 B760 B770 B791 B799 B803 B815  
B831 C000 C101 C106 C107 C108 C116  
C216 C316 C710 C800 C801 C802 C804  
C805 C806 C807 D010 D011 D012 D013  
D019 D020 D021 D022 D029 D040 D049  
D621 D622 E100 E199 E600 F010 F011  
F012 F013 F014 F015 F019 F020 F021  
F029 F211 F512 G001 G002 G010 G011  
G012 G013 G014 G015 G016 G019 G020  
G021 G022 G029 G030 G040 G050 G100  
G111 G112 G113 G221 G299 G553 G563  
H100 H101 H103 H141 H142 H201 H202  
H211 H401 H402 H441 H442 H521 H541  
H542 H543 H581 H582 H583 H600 H601  
H607 H608 H609 H621 H641 H642 H643  
H681 H682 H683 H685 H689 H715 H721  
H722 H723 J011 J012 J013 J111 J112  
J131 J132 J133 J151 J171 J172 J173  
J211 J241 J242 J271 J272 J411 J471  
J472 J490 J521 J581 J582 J598 J599  
K130 K199 K352 K399 K442 K499 K810

K830 K850 K899 L145 L352 L353 L355  
L399 L410 L420 L431 L499 L512 L531  
L532 L560 L599 L650 L941 L999 M111  
M112 M113 M114 M115 M116 M119 M121  
M122 M123 M124 M125 M126 M129 M131  
M132 M133 M135 M136 M139 M141 M143  
M144 M147 M148 M149 M150 M210 M211  
M212 M213 M214 M215 M216 M220 M221  
M222 M223 M224 M225 M226 M231 M232  
M233 M280 M311 M312 M313 M314 M315  
M316 M320 M321 M322 M323 M331 M332  
M333 M340 M342 M343 M344 M349 M382  
M391 M392 M393 M411 M510 M511 M512  
M513 M520 M521 M522 M523 M530 M531  
M532 M533 M540 M541 M610 M620 M630  
M781 Q454 R043 Markush Compounds  
012117313

## Chemical Indexing M3 \*22\*

Fragmentation Code A313 A331 A332  
A349 A350 A351 A382 A421 A422 A423  
A424 A425 A426 A427 A428 A430 A539  
A540 A541 A542 A544 A545 A546 A548  
A673 A676 A677 A678 A940 A960 A970  
B215 B305 B415 B434 B505 B515 B534  
B605 B615 B634 B701 B711 B712 B713  
B720 B741 B742 B751 B752 B760 B770  
B791 B799 B803 B809 B815 B831 B832  
B834 C000 C101 C106 C107 C108 C116  
C216 C316 C710 C800 C801 C802 C804  
C805 C806 C807 D010 D011 D012 D013  
D019 D020 D021 D022 D029 D040 D049  
D621 D622 E100 E199 E600 F010 F011  
F012 F013 F014 F015 F019 F020 F021  
F029 F211 F512 G001 G002 G010 G011  
G012 G013 G014 G015 G016 G019 G020  
G021 G022 G029 G030 G040 G050 G100  
G111 G112 G113 G221 G299 G553 G563

H100	H101	H103	H141	H142	H201	H202
H211	H401	H402	H441	H442	H521	H541
H542	H543	H581	H582	H583	H600	H601
H607	H608	H609	H621	H641	H642	H643
H681	H682	H683	H685	H689	H715	H721
H722	H723	J011	J012	J013	J111	J112
J131	J132	J133	J151	J171	J172	J173
J211	J241	J242	J271	J272	J411	J471
J472	J490	J521	J581	J582	J598	J599
K130	K199	K352	K399	K442	K499	K810
K830	K850	K899	L145	L352	L353	L355
L399	L410	L420	L431	L499	L512	L531
L532	L560	L599	L650	L941	L999	M111
M112	M113	M114	M115	M116	M119	M121
M122	M123	M124	M125	M126	M129	M131
M132	M133	M135	M136	M139	M141	M143
M144	M147	M148	M149	M150	M210	M211
M212	M213	M214	M215	M216	M220	M221
M222	M223	M224	M225	M226	M231	M232
M233	M280	M311	M312	M313	M314	M315
M316	M320	M321	M322	M323	M331	M332
M333	M340	M342	M343	M344	M349	M382
M391	M392	M393	M411	M510	M511	M512
M513	M520	M521	M522	M523	M530	M531
M532	M533	M540	M541	M610	M620	M630
M781	Q454	R043	Markush	Compounds		
01211	7314					

## Chemical Indexing M3 \*23\*

Fragmentation Code	A103	A111	A119			
A137	A155	A204	A212	A220	A238	A256
A400	A429	A500	A547	A600	A679	A700
A758	A759	A760	A761	A762	A763	A764
A765	A766	A767	A768	A769	A770	A771
A892	A940	A960	A970	B215	B415	B434
B505	B515	B534	B605	B615	B634	B701
B711	B712	B713	B720	B741	B742	B751
B752	B760	B770	B791	B799	B803	B815

B831	C000	C101	C106	C107	C108	C116
C216	C316	C710	C800	C801	C802	C804
C805	C806	C807	D000	D010	D011	D012
D013	D014	D015	D019	D020	D021	D022
D029	D040	D049	D621	D622	E350	E600
F010	F011	F012	F013	F014	F015	F019
F020	F021	F029	F211	F512	G001	G002
G010	G011	G012	G013	G014	G015	G016
G019	G020	G021	G022	G029	G030	G040
G050	G100	G111	G112	G113	G221	G299
G553	G563	H100	H101	H141	H142	H211
H401	H402	H441	H442	H521	H541	H542
H543	H581	H582	H583	H600	H601	H607
H608	H609	H621	H622	H623	H641	H642
H643	H681	H682	H683	H685	H689	H715
H721	H722	H723	J011	J012	J013	J111
J112	J131	J132	J133	J151	J171	J172
J173	J211	J241	J242	J271	J272	J411
J471	J472	J490	J521	J581	J582	J598
J599	K130	K199	K352	K399	K442	K499
K810	K830	K850	K899	L145	L352	L353
L355	L399	L410	L420	L431	L499	L512
L531	L532	L560	L599	L650	L941	L999
M111	M112	M113	M114	M115	M116	M119
M121	M122	M123	M124	M125	M126	M129
M131	M135	M136	M139	M141	M143	M144
M147	M148	M149	M150	M210	M211	M212
M213	M214	M215	M216	M220	M221	M222
M223	M224	M225	M226	M231	M232	M233
M280	M311	M312	M313	M314	M315	M316
M320	M321	M322	M323	M331	M332	M333
M340	M342	M343	M344	M349	M382	M391
M392	M393	M411	M510	M511	M512	M513
M520	M521	M522	M523	M530	M531	M532
M533	M540	M541	M620	M630	M781	Q454
R043	Ring Index Numbers					05479
Markush Compounds						012117315

## Chemical Indexing M3 \*24\*

Fragmentation Code A313 A331 A332  
A349 A350 A351 A382 A421 A422 A423  
A424 A425 A426 A427 A428 A430 A539  
A540 A541 A542 A544 A545 A546 A548  
A673 A676 A677 A678 A940 A960 A970  
B215 B305 B415 B434 B505 B515 B534  
B605 B615 B634 B701 B711 B712 B713  
B720 B741 B742 B751 B752 B760 B770  
B791 B799 B803 B809 B815 B831 B832  
B834 C000 C101 C106 C107 C108 C116  
C216 C316 C710 C800 C801 C802 C804  
C805 C806 C807 D000 D010 D011 D012  
D013 D014 D015 D019 D020 D021 D022  
D029 D040 D049 D621 D622 E350 E600  
F010 F011 F012 F013 F014 F015 F019  
F020 F021 F029 F211 F512 G001 G002  
G010 G011 G012 G013 G014 G015 G016  
G019 G020 G021 G022 G029 G030 G040  
G050 G100 G111 G112 G113 G221 G299  
G553 G563 H100 H101 H141 H142 H211  
H401 H402 H441 H442 H521 H541 H542  
H543 H581 H582 H583 H600 H601 H607  
H608 H609 H621 H622 H623 H641 H642  
H643 H681 H682 H683 H685 H689 H715  
H721 H722 H723 J011 J012 J013 J111  
J112 J131 J132 J133 J151 J171 J172  
J173 J211 J241 J242 J271 J272 J411  
J471 J472 J490 J521 J581 J582 J598  
J599 K130 K199 K352 K399 K442 K499  
K810 K830 K850 K899 L145 L352 L353  
L355 L399 L410 L420 L431 L499 L512  
L531 L532 L560 L599 L650 L941 L999  
M111 M112 M113 M114 M115 M116 M119  
M121 M122 M123 M124 M125 M126 M129  
M131 M135 M136 M139 M141 M143 M144  
M147 M148 M149 M150 M210 M211 M212  
M213 M214 M215 M216 M220 M221 M222

M223 M224 M225 M226 M231 M232 M233  
M280 M311 M312 M313 M314 M315 M316  
M320 M321 M322 M323 M331 M332 M333  
M340 M342 M343 M344 M349 M382 M391  
M392 M393 M411 M510 M511 M512 M513  
M520 M521 M522 M523 M530 M531 M532  
M533 M540 M541 M620 M630 M781 Q454  
R043 Ring Index Numbers 05479  
Markush Compounds 012117316

Chemical Indexing M3 \*25\*  
Fragmentation Code A103 A111 A119  
A137 A155 A204 A212 A220 A238 A256  
A400 A422 A423 A429 A500 A547 A600  
A679 A700 A758 A759 A760 A761 A762  
A763 A764 A765 A766 A767 A768 A769  
A770 A771 A892 A940 A960 A970 B215  
B415 B434 B505 B515 B534 B605 B615  
B634 B701 B711 B712 B713 B720 B741  
B742 B751 B752 B760 B770 B791 B799  
B803 B815 B831 C000 C101 C106 C107  
C108 C116 C216 C316 C550 C710 C720  
C801 C802 C804 C805 C807 D000 D010  
D011 D012 D013 D019 D020 D021 D022  
D029 D040 D049 D621 D622 E350 E600  
F010 F011 F012 F013 F014 F015 F019  
F020 F021 F029 F211 F512 G001 G002  
G010 G011 G012 G013 G014 G015 G016  
G019 G020 G021 G022 G029 G030 G040  
G050 G100 G111 G112 G113 G221 G299  
G553 G563 H100 H101 H141 H142 H211  
H401 H402 H441 H442 H521 H541 H542  
H543 H581 H582 H583 H600 H601 H607  
H608 H609 H621 H641 H642 H643 H681  
H682 H683 H685 H689 H715 H721 H722  
J011 J012 J013 J111 J112 J131 J132  
J133 J151 J171 J172 J173 J211 J241  
J242 J271 J272 J411 J471 J472 J490



J521 J581 J582 J598 J599 K130 K199  
K352 K399 K442 K499 K810 K830 K850  
K899 L145 L352 L353 L355 L399 L410  
L420 L431 L499 L512 L531 L532 L560  
L599 L650 L941 L999 M111 M112 M113  
M114 M115 M116 M119 M121 M122 M123  
M124 M125 M126 M129 M131 M135 M136  
M139 M141 M143 M144 M147 M148 M149  
M150 M210 M211 M212 M213 M214 M215  
M216 M220 M221 M222 M223 M224 M225  
M226 M231 M232 M233 M280 M311 M312  
M313 M314 M315 M316 M320 M321 M322  
M323 M331 M332 M333 M340 M342 M343  
M344 M349 M382 M391 M392 M393 M411  
M510 M511 M512 M513 M520 M521 M522  
M523 M530 M531 M532 M533 M540 M541  
M620 M630 M781 Q454 R043 Ring  
Index Numbers 07541 Markush  
Compounds 012117317

## Chemical Indexing M3 \*26\*

Fragmentation Code A313 A331 A332  
A349 A350 A351 A382 A421 A422 A423  
A424 A425 A426 A427 A428 A430 A539  
A540 A541 A542 A544 A545 A546 A548  
A673 A676 A677 A678 A940 A960 A970  
B215 B305 B415 B434 B505 B515 B534  
B605 B615 B634 B701 B711 B712 B713  
B720 B741 B742 B751 B752 B760 B770  
B791 B799 B803 B809 B815 B831 B832  
B834 C000 C101 C106 C107 C108 C116  
C216 C316 C550 C710 C720 C801 C802  
C804 C805 C807 D000 D010 D011 D012  
D013 D019 D020 D021 D022 D029 D040  
D049 D621 D622 E350 E600 F010 F011  
F012 F013 F014 F015 F019 F020 F021  
F029 F211 F512 G001 G002 G010 G011  
G012 G013 G014 G015 G016 G019 G020

G021	G022	G029	G030	G040	G050	G100
G111	G112	G113	G221	G299	G553	G563
H100	H101	H141	H142	H211	H401	H402
H441	H442	H521	H541	H542	H543	H581
H582	H583	H600	H601	H607	H608	H609
H621	H641	H642	H643	H681	H682	H683
H685	H689	H715	H721	H722	J011	J012
J013	J111	J112	J131	J132	J133	J151
J171	J172	J173	J211	J241	J242	J271
J272	J411	J471	J472	J490	J521	J581
J582	J598	J599	K130	K199	K352	K399
K442	K499	K810	K830	K850	K899	L145
L352	L353	L355	L399	L410	L420	L431
L499	L512	L531	L532	L560	L599	L650
L941	L999	M111	M112	M113	M114	M115
M116	M119	M121	M122	M123	M124	M125
M126	M129	M131	M135	M136	M139	M141
M143	M144	M147	M148	M149	M150	M210
M211	M212	M213	M214	M215	M216	M220
M221	M222	M223	M224	M225	M226	M231
M232	M233	M280	M311	M312	M313	M314
M315	M316	M320	M321	M322	M323	M331
M332	M333	M340	M342	M343	M344	M349
M382	M391	M392	M393	M411	M510	M511
M512	M513	M520	M521	M522	M523	M530
M531	M532	M533	M540	M541	M620	M630
M781	Q454	R043	Ring Index Numbers			
07541	Markush Compounds		01211	7318		

## Chemical Indexing M3 \*27\*

Fragmentation Code A103 A111 A119						
A137	A155	A204	A212	A220	A238	A256
A400	A429	A500	A547	A600	A679	A700
A758	A759	A760	A761	A762	A763	A764
A765	A766	A767	A768	A769	A770	A771
A892	A940	A960	A970	B215	B415	B434
B505	B515	B534	B605	B615	B634	B701
B711	B712	B713	B720	B741	B742	B751

B752	B760	B770	B791	B799	B803	B815
B831	C000	C101	C106	C107	C108	C116
C216	C316	C710	C800	C801	C802	C804
C805	C806	C807	D010	D011	D012	D013
D019	D020	D021	D022	D029	D040	D049
D621	D622	E600	F010	F011	F012	F013
F014	F015	F019	F020	F021	F029	F211
F512	G001	G002	G010	G011	G012	G013
G014	G015	G016	G019	G020	G021	G022
G029	G030	G040	G050	G100	G111	G112
G113	G221	G299	G553	G563	H100	H101
H103	H141	H142	H143	H211	H401	H402
H441	H442	H521	H541	H542	H543	H581
H582	H583	H600	H601	H607	H608	H609
H621	H641	H642	H643	H681	H682	H683
H685	H689	H715	H721	H722	H723	J011
J012	J013	J111	J112	J131	J132	J133
J151	J171	J172	J173	J211	J241	J242
J271	J272	J411	J471	J472	J490	J521
J581	J582	J598	J599	K130	K199	K352
K399	K442	K499	K810	K830	K850	K899
L145	L352	L353	L355	L399	L410	L420
L431	L499	L512	L531	L532	L560	L599
L650	L941	L999	M111	M112	M113	M114
M115	M116	M119	M121	M122	M123	M124
M125	M126	M129	M131	M135	M136	M139
M141	M143	M144	M147	M148	M149	M150
M210	M211	M212	M213	M214	M215	M216
M220	M221	M222	M223	M224	M225	M226
M231	M232	M233	M280	M311	M312	M313
M314	M315	M316	M320	M321	M322	M323
M331	M332	M333	M340	M342	M343	M344
M349	M382	M391	M392	M393	M411	M510
M511	M512	M513	M520	M521	M522	M523
M530	M531	M532	M533	M540	M541	M620
M630	M781	Q454	R043	Markush		
Compounds	012117319					

## Chemical Indexing M3 \*28\*

Fragmentation Code A313 A331 A332  
A349 A350 A351 A382 A421 A422 A423  
A424 A425 A426 A427 A428 A430 A539  
A540 A541 A542 A544 A545 A546 A548  
A673 A676 A677 A678 A940 A960 A970  
B215 B305 B415 B434 B505 B515 B534  
B605 B615 B634 B701 B711 B712 B713  
B720 B741 B742 B751 B752 B760 B770  
B791 B799 B803 B809 B815 B831 B832  
B834 C000 C101 C106 C107 C108 C116  
C216 C316 C710 C800 C801 C802 C804  
C805 C806 C807 D010 D011 D012 D013  
D019 D020 D021 D022 D029 D040 D049  
D621 D622 E600 F010 F011 F012 F013  
F014 F015 F019 F020 F021 F029 F211  
F512 G001 G002 G010 G011 G012 G013  
G014 G015 G016 G019 G020 G021 G022  
G029 G030 G040 G050 G100 G111 G112  
G113 G221 G299 G553 G563 H100 H101  
H103 H141 H142 H143 H211 H401 H402  
H441 H442 H521 H541 H542 H543 H581  
H582 H583 H600 H601 H607 H608 H609  
H621 H641 H642 H643 H681 H682 H683  
H685 H689 H715 H721 H722 H723 J011  
J012 J013 J111 J112 J131 J132 J133  
J151 J171 J172 J173 J211 J241 J242  
J271 J272 J411 J471 J472 J490 J521  
J581 J582 J598 J599 K130 K199 K352  
K399 K442 K499 K810 K830 K850 K899  
L145 L352 L353 L355 L399 L410 L420  
L431 L499 L512 L531 L532 L560 L599  
L650 L941 L999 M111 M112 M113 M114  
M115 M116 M119 M121 M122 M123 M124  
M125 M126 M129 M131 M135 M136 M139  
M141 M143 M144 M147 M148 M149 M150  
M210 M211 M212 M213 M214 M215 M216  
M220 M221 M222 M223 M224 M225 M226

M231 M232 M233 M280 M311 M312 M313  
M314 M315 M316 M320 M321 M322 M323  
M331 M332 M333 M340 M342 M343 M344  
M349 M382 M391 M392 M393 M411 M510  
M511 M512 M513 M520 M521 M522 M523  
M530 M531 M532 M533 M540 M541 M620  
M630 M781 Q454 R043 Markush  
Compounds 012117320

## Chemical Indexing M3 \*29\*

Fragmentation Code A103 A111 A119  
A137 A155 A204 A212 A220 A238 A256  
A400 A429 A500 A547 A600 A679 A700  
A758 A759 A760 A761 A762 A763 A764  
A765 A766 A767 A768 A769 A770 A771  
A892 A940 A960 A970 B415 B434 B505  
B515 B534 B605 B615 B634 B701 B711  
B712 B713 B720 B741 B742 B743 B751  
B760 B770 B791 B799 B803 B815 B831  
B832 B834 C000 C101 C106 C107 C108  
C116 C216 C316 C710 C800 C801 C802  
C804 C805 C806 C807 D000 D011 D012  
D013 D021 D022 D023 D029 D621 D622  
E100 E600 F011 F012 F013 F014 F015  
F211 F512 G001 G002 G020 G021 G022  
G029 G031 G038 G039 G040 G041 G050  
G310 G399 G553 G563 H100 H101 H102  
H103 H121 H141 H142 H143 H181 H201  
H211 H401 H402 H441 H442 H521 H541  
H542 H543 H581 H582 H583 H600 H601  
H607 H608 H609 H621 H622 H641 H642  
H643 H681 H682 H683 H685 H689 H713  
H715 H716 H721 H722 H723 J011 J012  
J013 J111 J112 J131 J132 J133 J151  
J171 J172 J173 J211 J241 J242 J271  
J272 J411 J471 J472 J490 J521 J581  
J582 J598 J599 K130 K199 K352 K399  
K441 K442 K499 K810 K830 K850 K899

L145 L352 L353 L355 L399 L410 L420  
L431 L499 L512 L531 L532 L560 L599  
L650 L941 L999 M111 M112 M113 M114  
M115 M116 M119 M121 M122 M123 M124  
M125 M126 M129 M131 M135 M136 M139  
M141 M142 M143 M144 M147 M148 M149  
M150 M210 M211 M212 M213 M214 M215  
M216 M220 M221 M222 M223 M224 M225  
M226 M231 M232 M233 M280 M311 M312  
M313 M314 M315 M316 M320 M321 M322  
M323 M331 M332 M333 M340 M342 M343  
M344 M349 M382 M391 M392 M393 M411  
M510 M511 M520 M521 M530 M531 M532  
M540 M620 M630 M781 Q454 R043 Ring  
Index Numbers 06706 Markush  
Compounds 012117321

Chemical Indexing M3 \*30\*  
Fragmentation Code A313 A331 A332  
A349 A350 A351 A382 A421 A422 A423  
A424 A425 A426 A427 A428 A430 A539  
A540 A541 A542 A544 A545 A546 A548  
A673 A676 A677 A678 A940 A960 A970  
B215 B305 B415 B434 B505 B515 B534  
B605 B615 B634 B701 B711 B712 B713  
B720 B741 B742 B743 B751 B752 B760  
B770 B791 B799 B803 B809 B815 B831  
B832 B834 C000 C101 C106 C107 C108  
C116 C216 C316 C710 C800 C801 C802  
C804 C805 C806 C807 D000 D011 D012  
D013 D021 D022 D023 D029 D621 D622  
E100 E600 F011 F012 F013 F014 F015  
F211 F512 G001 G002 G020 G021 G022  
G029 G031 G038 G039 G040 G041 G050  
G310 G399 G553 G563 H100 H101 H102  
H103 H121 H141 H142 H143 H181 H201  
H211 H401 H402 H441 H442 H521 H541  
H542 H543 H581 H582 H583 H600 H601

H607 H608 H609 H621 H622 H641 H642  
H643 H681 H682 H683 H685 H689 H713  
H715 H716 H721 H722 H723 J011 J012  
J013 J111 J112 J131 J132 J133 J151  
J171 J172 J173 J211 J241 J242 J271  
J272 J411 J471 J472 J490 J521 J581  
J582 J598 J599 K130 K199 K352 K399  
K441 K442 K499 K810 K830 K850 K899  
L145 L352 L353 L355 L399 L410 L420  
L431 L499 L512 L531 L532 L560 L599  
L650 L941 L999 M111 M112 M113 M114  
M115 M116 M119 M121 M122 M123 M124  
M125 M126 M129 M131 M135 M136 M139  
M141 M142 M143 M144 M147 M148 M149  
M150 M210 M211 M212 M213 M214 M215  
M216 M220 M221 M222 M223 M224 M225  
M226 M231 M232 M233 M280 M311 M312  
M313 M314 M315 M316 M320 M321 M322  
M323 M331 M332 M333 M340 M342 M343  
M344 M349 M382 M391 M392 M393 M411  
M510 M511 M520 M521 M530 M531 M532  
M540 M620 M630 M781 Q454 R043 Ring  
Index Numbers 06706 Markush  
Compounds 012117322

Chemical Indexing M3 \*31\*  
Fragmentation Code A103 A111 A119  
A137 A155 A204 A212 A220 A238 A256  
A400 A429 A500 A547 A600 A679 A700  
A758 A759 A760 A761 A762 A763 A764  
A765 A766 A767 A768 A769 A770 A771  
A892 A940 A960 A970 B215 B415 B434  
B505 B515 B534 B605 B615 B634 B701  
B711 B712 B713 B720 B741 B742 B751  
B752 B760 B770 B791 B799 B803 B815  
B831 C000 C101 C106 C107 C108 C116  
C216 C316 C710 C800 C801 C802 C804  
C805 C806 C807 D010 D011 D012 D013

D019	D020	D021	D022	D029	D040	D049
D621	D622	E600	F010	F011	F012	F013
F014	F015	F019	F020	F021	F029	F211
F512	G001	G002	G010	G011	G012	G013
G014	G015	G016	G019	G020	G021	G022
G029	G030	G040	G050	G100	G111	G112
G113	G221	G299	G331	G399	G553	G563
H100	H101	H141	H142	H211	H401	H402
H441	H442	H521	H541	H542	H543	H581
H582	H583	H600	H601	H607	H608	H609
H621	H641	H642	H643	H681	H682	H683
H685	H689	H713	H715	H716	H721	H722
H723	J011	J012	J013	J111	J112	J131
J132	J133	J151	J171	J172	J173	J211
J241	J242	J271	J272	J411	J471	J472
J490	J521	J581	J582	J598	J599	K122
K130	K199	K352	K399	K442	K499	K810
K830	K850	K899	L145	L352	L353	L355
L399	L410	L420	L431	L499	L512	L531
L532	L560	L599	L650	L941	L999	M111
M112	M113	M114	M115	M116	M119	M121
M122	M123	M124	M125	M126	M129	M131
M132	M135	M136	M139	M141	M142	M143
M144	M147	M148	M149	M150	M210	M211
M212	M213	M214	M215	M216	M220	M221
M222	M223	M224	M225	M226	M231	M232
M233	M280	M311	M312	M313	M314	M315
M316	M320	M321	M322	M323	M331	M332
M333	M334	M340	M342	M343	M344	M349
M382	M391	M392	M393	M411	M510	M511
M512	M513	M520	M521	M522	M523	M530
M531	M532	M533	M540	M541	M620	M630
M781	Q454	R043	Markush	Compounds		
01211	7323					

Chemical Indexing M3 \*32\*

Fragmentation Code A313 A331 A332

A349 A350 A351 A382 A421 A422 A423



A424	A425	A426	A427	A428	A430	A539
A540	A541	A542	A544	A545	A546	A548
A673	A676	A677	A678	A940	A960	A970
B215	B305	B415	B434	B505	B515	B534
B605	B615	B634	B701	B711	B712	B713
B720	B741	B742	B751	B752	B760	B770
B791	B799	B803	B809	B815	B831	B832
B834	C000	C101	C106	C107	C108	C116
C216	C316	C710	C800	C801	C802	C804
C805	C806	C807	D010	D011	D012	D013
D019	D020	D021	D022	D029	D040	D049
D621	D622	E600	F010	F011	F012	F013
F014	F015	F019	F020	F021	F029	F211
F512	G001	G002	G010	G011	G012	G013
G014	G015	G016	G019	G020	G021	G022
G029	G030	G040	G050	G100	G111	G112
G113	G221	G299	G331	G399	G553	G563
H100	H101	H141	H142	H211	H401	H402
H441	H442	H521	H541	H542	H543	H581
H582	H583	H600	H601	H607	H608	H609
H621	H641	H642	H643	H681	H682	H683
H685	H689	H713	H715	H716	H721	H722
H723	J011	J012	J013	J111	J112	J131
J132	J133	J151	J171	J172	J173	J211
J241	J242	J271	J272	J411	J471	J472
J490	J521	J581	J582	J598	J599	K122
K130	K199	K352	K399	K442	K499	K810
K830	K850	K899	L145	L352	L353	L355
L399	L410	L420	L431	L499	L512	L531
L532	L560	L599	L650	L941	L999	M111
M112	M113	M114	M115	M116	M119	M121
M122	M123	M124	M125	M126	M129	M131
M132	M135	M136	M139	M141	M142	M143
M144	M147	M148	M149	M150	M210	M211
M212	M213	M214	M215	M216	M220	M221
M222	M223	M224	M225	M226	M231	M232
M233	M280	M311	M312	M313	M314	M315
M316	M320	M321	M322	M323	M331	M332

M333 M334 M340 M342 M343 M344 M349  
M382 M391 M392 M393 M411 M510 M511  
M512 M513 M520 M521 M522 M523 M530  
M531 M532 M533 M540 M541 M620 M630  
M781 Q454 R043 Markush Compounds  
012117324

## Chemical Indexing M3 \*33\*

Fragmentation Code A103 A111 A119  
A137 A155 A204 A212 A220 A238 A256  
A400 A429 A500 A600 A679 A700 A758  
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B815 B831 B832 B834 C000 C101 C106  
C107 C108 C116 C216 C316 C710 C800  
C801 C802 C804 C805 C806 C807 D010  
D011 D012 D013 D019 D020 D021 D022  
D029 D040 D049 D621 D622 E600 F010  
F011 F012 F013 F014 F015 F019 F020  
F021 F029 F211 F512 G001 G002 G010  
G011 G012 G013 G014 G015 G016 G019  
G020 G021 G022 G029 G030 G040 G050  
G100 G111 G112 G113 G221 G299 G553  
G563 H100 H101 H141 H142 H211 H401  
H402 H441 H442 H521 H541 H542 H543  
H581 H582 H583 H600 H601 H607 H608  
H609 H621 H641 H642 H643 H681 H682  
H683 H685 H689 H715 H721 H722 H723  
J011 J012 J013 J111 J112 J131 J132  
J133 J151 J171 J172 J173 J211 J241  
J242 J271 J272 J411 J471 J472 J490  
J521 J581 J582 J598 J599 K130 K199  
K352 K399 K442 K499 K810 K830 K850  
K899 L145 L352 L353 L355 L399 L410

L420 L431 L499 L512 L531 L532 L560  
L599 L650 L941 L999 M111 M112 M113  
M114 M115 M116 M119 M121 M122 M123  
M124 M125 M126 M129 M131 M135 M136  
M139 M141 M143 M144 M147 M148 M149  
M150 M210 M211 M212 M213 M214 M215  
M216 M220 M221 M222 M223 M224 M225  
M226 M231 M232 M233 M280 M311 M312  
M313 M314 M315 M316 M320 M321 M322  
M323 M331 M332 M333 M340 M342 M343  
M344 M349 M382 M391 M392 M393 M411  
M510 M511 M512 M513 M520 M521 M522  
M523 M530 M531 M532 M533 M540 M541  
M620 M630 M781 Q454 R043 Markush  
Compounds 012117325

## Chemical Indexing M3 \*34\*

Fragmentation Code A313 A331 A332  
A349 A350 A351 A382 A421 A422 A423  
A424 A425 A426 A427 A428 A430 A539  
A540 A541 A542 A544 A545 A546 A548  
A673 A676 A677 A678 A940 A960 A970  
B215 B305 B415 B434 B505 B515 B534  
B605 B615 B634 B701 B711 B712 B713  
B720 B730 B741 B742 B743 B751 B752  
B760 B770 B791 B799 B803 B809 B815  
B831 B832 B834 C000 C101 C106 C107  
C108 C116 C216 C316 C710 C800 C801  
C802 C804 C805 C806 C807 D010 D011  
D012 D013 D019 D020 D021 D022 D029  
D040 D049 D621 D622 E600 F010 F011  
F012 F013 F014 F015 F019 F020 F021  
F029 F211 F512 G001 G002 G010 G011  
G012 G013 G014 G015 G016 G019 G020  
G021 G022 G029 G030 G040 G050 G100  
G111 G112 G113 G221 G299 G553 G563  
H100 H101 H141 H142 H211 H401 H402  
H441 H442 H521 H541 H542 H543 H581

H582	H583	H600	H601	H607	H608	H609
H621	H641	H642	H643	H681	H682	H683
H685	H689	H715	H721	H722	H723	J011
J012	J013	J111	J112	J131	J132	J133
J151	J171	J172	J173	J211	J241	J242
J271	J272	J411	J471	J472	J490	J521
J581	J582	J598	J599	K130	K199	K352
K399	K442	K499	K810	K830	K850	K899
L145	L352	L353	L355	L399	L410	L420
L431	L499	L512	L531	L532	L560	L599
L650	L941	L999	M111	M112	M113	M114
M115	M116	M119	M121	M122	M123	M124
M125	M126	M129	M131	M135	M136	M139
M141	M143	M144	M147	M148	M149	M150
M210	M211	M212	M213	M214	M215	M216
M220	M221	M222	M223	M224	M225	M226
M231	M232	M233	M280	M311	M312	M313
M314	M315	M316	M320	M321	M322	M323
M331	M332	M333	M340	M342	M343	M344
M349	M382	M391	M392	M393	M411	M510
M511	M512	M513	M520	M521	M522	M523
M530	M531	M532	M533	M540	M541	M620
M630	M781	Q454	R043	Markush		
Compounds	012117326					

## Chemical Indexing M3 \*35\*

Fragmentation Code	A103	A111	A119			
A137	A155	A204	A212	A220	A238	A256
A400	A429	A500	A547	A600	A679	A700
A758	A759	A760	A761	A762	A763	A764
A765	A766	A767	A768	A769	A770	A771
A892	A940	A960	A970	B215	B415	B434
B505	B515	B534	B605	B615	B634	B701
B711	B712	B713	B720	B741	B742	B751
B752	B760	B770	B791	B799	B803	B815
B831	C000	C101	C106	C107	C108	C116
C216	C316	C710	C800	C801	C802	C804
C805	C806	C807	D000	D010	D011	D012

D013 D019 D020 D021 D022 D023 D029  
D040 D049 D120 D210 D621 D622 E400  
E600 F010 F011 F012 F013 F014 F015  
F019 F020 F021 F029 F211 F512 G001  
G002 G010 G011 G012 G013 G014 G015  
G016 G019 G020 G021 G022 G029 G030  
G040 G050 G100 G111 G112 G113 G221  
G299 G553 G563 H100 H101 H102 H103  
H141 H142 H211 H401 H402 H441 H442  
H521 H541 H542 H543 H581 H582 H583  
H600 H601 H607 H608 H609 H621 H641  
H642 H643 H681 H682 H683 H685 H689  
H715 H721 H722 J011 J012 J013 J111  
J112 J131 J132 J133 J151 J171 J172  
J173 J211 J241 J242 J271 J272 J411  
J471 J472 J490 J521 J581 J582 J598  
J599 K130 K199 K352 K399 K442 K499  
K810 K830 K850 K899 L145 L352 L353  
L355 L399 L410 L420 L431 L499 L512  
L531 L532 L560 L599 L650 L941 L942  
L999 M111 M112 M113 M114 M115 M116  
M119 M121 M122 M123 M124 M125 M126  
M129 M131 M135 M136 M139 M141 M143  
M144 M147 M148 M149 M150 M210 M211  
M212 M213 M214 M215 M216 M220 M221  
M222 M223 M224 M225 M226 M231 M232  
M233 M280 M311 M312 M313 M314 M315  
M316 M320 M321 M322 M323 M331 M332  
M333 M340 M342 M343 M344 M349 M382  
M391 M392 M393 M411 M510 M511 M512  
M513 M520 M521 M522 M523 M530 M531  
M532 M533 M540 M541 M620 M630 M781  
Q454 R043 Markush Compounds  
012117327

Chemical Indexing M3 \*36\*  
Fragmentation Code A313 A331 A332  
A349 A350 A351 A382 A421 A422 A423

A424	A425	A426	A427	A428	A430	A539
A540	A541	A542	A544	A545	A546	A548
A673	A676	A677	A678	A940	A960	A970
B215	B305	B415	B434	B505	B515	B534
B605	B615	B634	B701	B711	B712	B713
B720	B741	B742	B751	B752	B760	B770
B791	B799	B803	B809	B815	B831	B832
B834	C000	C101	C106	C107	C108	C116
C216	C316	C710	C800	C801	C802	C804
C805	C806	C807	D000	D010	D011	D012
D013	D019	D020	D021	D022	D023	D029
D040	D049	D120	D210	D621	D622	E400
E600	F010	F011	F012	F013	F014	F015
F019	F020	F021	F029	F211	F512	G001
G002	G010	G011	G012	G013	G014	G015
G016	G019	G020	G021	G022	G029	G030
G040	G050	G100	G111	G112	G113	G221
G299	G553	G563	H100	H101	H102	H103
H141	H142	H211	H401	H402	H441	H442
H521	H541	H542	H543	H581	H582	H583
H600	H601	H607	H608	H609	H621	H641
H642	H643	H681	H682	H683	H685	H689
H715	H721	H722	J011	J012	J013	J111
J112	J131	J132	J133	J151	J171	J172
J173	J211	J241	J242	J271	J272	J411
J471	J472	J490	J521	J581	J582	J598
J599	K130	K199	K352	K399	K442	K499
K810	K830	K850	K899	L145	L352	L353
L355	L399	L410	L420	L431	L499	L512
L531	L532	L560	L599	L650	L941	L942
L999	M111	M112	M113	M114	M115	M116
M119	M121	M122	M123	M124	M125	M126
M129	M131	M135	M136	M139	M141	M143
M144	M147	M148	M149	M150	M210	M211
M212	M213	M214	M215	M216	M220	M221
M222	M223	M224	M225	M226	M231	M232
M233	M280	M311	M312	M313	M314	M315
M316	M320	M321	M322	M323	M331	M332

M333 M340 M342 M343 M344 M349 M382  
M391 M392 M393 M411 M510 M511 M512  
M513 M520 M521 M522 M523 M530 M531  
M532 M533 M540 M541 M620 M630 M781  
Q454 R043 Markush Compounds  
012117328

## Chemical Indexing M3 \*37\*

Fragmentation Code A103 A111 A119  
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A765 A766 A767 A768 A769 A770 A771  
A892 A940 A960 A970 B415 B434 B505  
B515 B534 B605 B615 B634 B701 B711  
B712 B713 B720 B741 B742 B751 B760  
B770 B791 B799 B803 B815 B831 C000  
C101 C106 C107 C108 C116 C216 C316  
C710 C800 C801 C802 C804 C805 C806  
C807 D010 D011 D012 D013 D014 D019  
D020 D021 D022 D029 D040 D049 D621  
D622 E250 E600 F010 F011 F012 F013  
F014 F015 F019 F020 F021 F029 F211  
F512 G001 G002 G010 G011 G012 G013  
G014 G015 G016 G019 G020 G021 G022  
G029 G030 G040 G050 G100 G111 G112  
G113 G221 G299 G553 G563 H100 H101  
H141 H142 H211 H212 H401 H402 H441  
H442 H521 H541 H542 H543 H581 H582  
H583 H600 H601 H607 H608 H609 H621  
H641 H642 H643 H681 H682 H683 H685  
H689 H713 H715 H716 H721 H722 J011  
J012 J013 J111 J112 J131 J132 J133  
J151 J171 J172 J173 J211 J241 J242  
J271 J272 J411 J471 J472 J490 J521  
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K899 L145 L352 L353 L355 L399 L410

L420 L431 L499 L512 L531 L532 L560  
L599 L650 L930 L941 L999 M111 M112  
M113 M114 M115 M116 M119 M121 M122  
M123 M124 M125 M126 M129 M131 M135  
M136 M139 M141 M143 M144 M147 M148  
M149 M150 M210 M211 M212 M213 M214  
M215 M216 M220 M221 M222 M223 M224  
M225 M226 M231 M232 M233 M280 M311  
M312 M313 M314 M315 M316 M320 M321  
M322 M323 M331 M332 M333 M340 M342  
M343 M344 M349 M382 M391 M392 M393  
M411 M510 M511 M512 M513 M520 M521  
M522 M523 M530 M531 M532 M533 M540  
M541 M620 M630 M781 Q454 R043 Ring  
Index Numbers 02448 Markush  
Compounds 012117329

Chemical Indexing M3 \*38\*  
Fragmentation Code A313 A331 A332  
A349 A350 A351 A382 A421 A422 A423  
A424 A425 A426 A427 A428 A430 A539  
A540 A541 A542 A544 A545 A546 A548  
A673 A676 A677 A678 A940 A960 A970  
B215 B305 B415 B434 B505 B515 B534  
B605 B615 B634 B701 B711 B712 B713  
B720 B741 B742 B751 B752 B760 B770  
B791 B799 B803 B809 B815 B831 B832  
B834 C000 C101 C106 C107 C108 C116  
C216 C316 C710 C800 C801 C802 C804  
C805 C806 C807 D010 D011 D012 D013  
D014 D019 D020 D021 D022 D029 D040  
D049 D621 D622 E250 E600 F010 F011  
F012 F013 F014 F015 F019 F020 F021  
F029 F211 F512 G001 G002 G010 G011  
G012 G013 G014 G015 G016 G019 G020  
G021 G022 G029 G030 G040 G050 G100  
G111 G112 G113 G221 G299 G553 G563  
H100 H101 H141 H142 H211 H212 H401



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H581 H582 H583 H600 H601 H607 H608  
H609 H621 H641 H642 H643 H681 H682  
H683 H685 H689 H713 H715 H716 H721  
H722 J011 J012 J013 J111 J112 J131  
J132 J133 J151 J171 J172 J173 J211  
J241 J242 J271 J272 J411 J471 J472  
J490 J521 J523 J581 J582 J598 J599  
K130 K199 K352 K399 K442 K499 K810  
K830 K850 K899 L145 L352 L353 L355  
L399 L410 L420 L431 L499 L512 L531  
L532 L560 L599 L650 L930 L941 L999  
M111 M112 M113 M114 M115 M116 M119  
M121 M122 M123 M124 M125 M126 M129  
M131 M135 M136 M139 M141 M143 M144  
M147 M148 M149 M150 M210 M211 M212  
M213 M214 M215 M216 M220 M221 M222  
M223 M224 M225 M226 M231 M232 M233  
M280 M311 M312 M313 M314 M315 M316  
M320 M321 M322 M323 M331 M332 M333  
M340 M342 M343 M344 M349 M382 M391  
M392 M393 M411 M510 M511 M512 M513  
M520 M521 M522 M523 M530 M531 M532  
M533 M540 M541 M620 M630 M781 Q454  
R043 Ring Index Numbers 02448  
Markush Compounds 012117330

Chemical Indexing M3 \*39\*  
Fragmentation Code A103 A111 A119  
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B505 B515 B534 B605 B615 B634 B701  
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B831 C000 C101 C106 C107 C108 C116

C216 C316 C710 C800 C801 C802 C804  
C805 C806 C807 D010 D011 D012 D013  
D019 D020 D021 D022 D029 D040 D049  
D420 D621 D622 E600 F010 F011 F012  
F013 F014 F015 F019 F020 F021 F029  
F211 F512 G001 G002 G010 G011 G012  
G013 G014 G015 G016 G019 G020 G021  
G022 G029 G030 G040 G050 G100 G111  
G112 G113 G221 G299 G553 G563 H100  
H101 H141 H142 H211 H401 H402 H441  
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H583 H600 H601 H607 H608 H609 H621  
H641 H642 H643 H681 H682 H683 H685  
H689 H715 H721 H722 H723 J011 J012  
J013 J111 J112 J131 J132 J133 J151  
J171 J172 J173 J211 J241 J242 J271  
J272 J411 J471 J472 J490 J521 J581  
J582 J598 J599 K130 K199 K352 K399  
K441 K442 K499 K810 K830 K850 K899  
L145 L352 L353 L355 L399 L410 L420  
L431 L499 L512 L531 L532 L560 L599  
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M141 M143 M144 M147 M148 M149 M150  
M210 M211 M212 M213 M214 M215 M216  
M220 M221 M222 M223 M224 M225 M226  
M231 M232 M233 M280 M311 M312 M313  
M314 M315 M316 M320 M321 M322 M323  
M331 M332 M333 M340 M342 M343 M344  
M349 M382 M391 M392 M393 M411 M510  
M511 M512 M513 M520 M521 M522 M523  
M530 M531 M532 M533 M540 M541 M620  
M630 M781 Q454 R043 Ring Index  
Numbers 05974 Markush Compounds  
012117331

Chemical Indexing M3 \*40\*

Fragmentation Code				A313	A331	A332
A349	A350	A351	A382	A421	A422	A423
A424	A425	A426	A427	A428	A430	A539
A540	A541	A542	A544	A545	A546	A548
A673	A676	A677	A678	A940	A960	A970
B215	B305	B415	B434	B505	B515	B534
B605	B615	B634	B701	B711	B712	B713
B720	B741	B742	B751	B752	B760	B770
B791	B799	B803	B809	B815	B831	B832
B834	C000	C101	C106	C107	C108	C116
C216	C316	C710	C800	C801	C802	C804
C805	C806	C807	D010	D011	D012	D013
D019	D020	D021	D022	D029	D040	D049
D420	D621	D622	E600	F010	F011	F012
F013	F014	F015	F019	F020	F021	F029
F211	F512	G001	G002	G010	G011	G012
G013	G014	G015	G016	G019	G020	G021
G022	G029	G030	G040	G050	G100	G111
G112	G113	G221	G299	G553	G563	H100
H101	H141	H142	H211	H401	H402	H441
H442	H521	H541	H542	H543	H581	H582
H583	H600	H601	H607	H608	H609	H621
H641	H642	H643	H681	H682	H683	H685
H689	H715	H721	H722	H723	J011	J012
J013	J111	J112	J131	J132	J133	J151
J171	J172	J173	J211	J241	J242	J271
J272	J411	J471	J472	J490	J521	J581
J582	J598	J599	K130	K199	K352	K399
K441	K442	K499	K810	K830	K850	K899
L145	L352	L353	L355	L399	L410	L420
L431	L499	L512	L531	L532	L560	L599
L650	L941	L999	M111	M112	M113	M114
M115	M116	M119	M121	M122	M123	M124
M125	M126	M129	M131	M135	M136	M139
M141	M143	M144	M147	M148	M149	M150
M210	M211	M212	M213	M214	M215	M216
M220	M221	M222	M223	M224	M225	M226
M231	M232	M233	M280	M311	M312	M313

M314 M315 M316 M320 M321 M322 M323  
M331 M332 M333 M340 M342 M343 M344  
M349 M382 M391 M392 M393 M411 M510  
M511 M512 M513 M520 M521 M522 M523  
M530 M531 M532 M533 M540 M541 M620  
M630 M781 Q454 R043 Ring Index  
Numbers 05974 Markush Compounds  
012117332

Chemical Indexing M3 \*41\*  
Fragmentation Code A400 A500 A600  
A700 A960 A970 B605 B720 B732 B770  
B803 B831 C000 C800 C801 C802 C803  
C804 C805 C806 C807 D010 D019 D020  
D029 D040 D049 F010 F011 F019 F020  
F021 F029 F511 F599 G001 G002 G010  
G011 G012 G013 G019 G020 G021 G022  
G029 G040 G100 G111 G112 G221 G299  
H213 H600 H601 H608 H609 H681 H682  
H683 H689 J471 J472 J581 J582 L512  
L599 M121 M122 M123 M124 M125 M126  
M129 M135 M139 M210 M211 M212 M213  
M214 M215 M216 M220 M221 M222 M223  
M224 M225 M226 M231 M232 M233 M262  
M280 M281 M282 M311 M312 M313 M314  
M315 M316 M320 M321 M322 M323 M331  
M332 M333 M340 M342 M343 M349 M362  
M372 M382 M391 M392 M393 M411 M510  
M511 M512 M513 M520 M521 M522 M523  
M530 M531 M532 M533 M540 M620 M630  
M781 Q454 R043 Markush Compounds  
012117333

**UNLINKED-DERWENT-REGISTRY-NUMBERS:** ; 1164U

**SECONDARY-ACC-NO:**

**CPI Secondary Accession Numbers:** 2004-057734

**Non-CPI Secondary Accession Numbers:** 2004-114077